CFD Modeling of Hydrogen Releases and Dispersion in Hydrogen Energy Station

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Abstract

This paper presents the results of computational fluid dynamics (CFD) modeling of hydrogen releases and dispersion in simple geometries and a real industrial environment. 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 for simple geometries were compared with the published data on hydrogen dispersion. The similarity study of helium and hydrogen releases has been conducted. Numerical results on hydrogen concentration predictions were obtained in the real industrial environment, which is a hydrogen energy station (HES) produced by Stuart Energy Systems Corporation. The CFD modeling was then applied to the risk assessment under hypothetical failure hydrogen leak scenarios in the HES. CFD modeling has proven to be a reliable, effective and relatively inexpensive tool to evaluate the effects of hydrogen leaks in the HES.

Keywords: CFD modeling, gas release, gas dispersion, PHOENICS, hydrogen, numerical simulation, scaling analysis.

1. Introduction

Stuart Energy Systems Corporation has installed a Hydrogen Energy Station (HES) for both vehicle fueling and power applications. The station produces and stores hydrogen for generating back-up power in the event of a grid power disruption. It also supplies additional primary power to the Stuart Energy building during normal operation or during peak-demand times. In addition, it is capable of dispensing clean hydrogen fuel to vehicles and can support a small fleet of vehicles. Power components of HES form so-called Hydrogen Backup Power System or Alpha H2BPS, which contains hydrogen generator, storage, internal combustion engines, ventilation duct, exhaust fan, industrial unit heater and hydrogen sensors.

The electrolyser in the hydrogen generator (CFA 450) passes an electric current through water separating it into its essential elements, oxygen and hydrogen. The hydrogen is compressed in CFA 450 and sent to the storage room until it is used to fuel vehicles or delivered to the internal combustion engines (ICEs) to create electricity. An industrial unit heater hung from the ceiling maintains the room temperature within a certain level (about 20ºC). The generator room is well ventilated by the ventilation duct and exhaust fan when the ICEs are working.

The exhaust fan, which is assembled on the roof, circulates the exhaust air at a flow rate of 10,000 CFM (4.72m^3/s) from the room to the outside atmosphere, and the duct makes up fresh air to the room through the penthouse air louvers located on the roof. When either of the two ICE is working, 2,725 CFM (1.29 m^3/s) room air is sucked into the working ICE and all the exhaust gas produced by the ICE is assumed to be released to the outside atmosphere through the muffler and the louvers attached to the radiators. When no ICE is working, both the penthouse duct and the exhaust fan are closed but can be opened due to the activation of temperature sensors or hydrogen sensors placed in the room. The Gen-set structures include two supporting columns and Gen-set platform, where the two ICEs are installed. The reader is referred to figure 4 for detailed installation diagram.

Hydrogen may release from any broken valve, piping, storage, muffler, ICE or venting stack, resulting in a complicated 3-D transient gas mixture behaviour, represented by a LFL (4.1% vol.) hydrogen cloud under different real working conditions. To assess the effectiveness of selected hydrogen sensor locations and ventilation design, as well as catastrophic hydrogen leak risks inside the HES (Alpha H2BPS) room, a CFD model of hydrogen release and dispersion has been developed, using PHOENICS [1], a well-recognized general-purpose CFD software package that has been validated and successfully used around the world for more than 20 years.

The CFD model was first validated through comparing the numerical results for a simple geometry (hallway) with the published data [2]. Then the similarity of helium and hydrogen releases was studied. Finally, the model was applied to the simulations of catastrophic hydrogen release in the Alpha H2BPS generator room under real industrial working scenarios with a real geometry and boundary conditions. The numerical results were used to assess the hydrogen risks in the HES room as well as to optimize the ventilation design.

2. Mathematical model

Transient hydrogen leaks are governed by the momentum equations, the continuity equation and the hydrogen mass conservation equation. The governing equations are expressed in summation notation as [3]:

Momentum Equations: $$\frac{\partial(ru_i)}{\partial t} + u_j\frac{\partial(ru_i)}{\partial x_j} = -\frac{\partial P}{\partial x_j} + rf_i + \frac{\partial}{\partial x_j}\left(m\frac{\partial u_i}{\partial x_j}\right), \quad (1)$$

Continuity Equation: $$\frac{\partial r}{\partial t} + \frac{\partial(ru_i)}{\partial x_i} = 0, \quad (2)$$

Hydrogen Mass Conservation Equation: $$\frac{\partial(rC)}{\partial t} + u_j\frac{\partial(rC)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[D\frac{\partial(rC)}{\partial x_j}\right] + C'', \quad (3)$$

where x_1, x_2 and x_3 denote the Cartesian coordinates; u_1, u_2 and u_3 are the velocity components; f_i $(i = 1,2,3)$ is the body force in the x_i direction; P is the gas mixture pressure; C is the mass concentration of hydrogen; C'' is the hydrogen source; D is the hydrogen diffusion coefficient in air; r and m are the gas mixture density and its laminar viscosity, which are dependent on the hydrogen mass concentration C or the hydrogen volumetric concentration a :

$$r = \frac{P}{[CR_{H_2} + (1-C)R_{air}]T}, \quad m = m_{H_2} a + m_{air}(1-a), \quad a = \frac{CR_{H_2}}{CR_{H_2} + (1-C)R_{air}} \qquad (4)$$

Here, T is the absolute temperature; R_{H_2} and R_{air} are the gas constants of hydrogen and air, respectively. The difference between the gas mixture density and the air density accounts for the buoyancy force represented by $rf_3 = (r - r_{air})g$ in the x_3 direction (vertical direction).

The equations (4) for the mixture density, laminar viscosity and volume fraction were incorporated into the continuity, momentum and mass diffusion equations of PHOENICS through the user-defined functions. The LVEL turbulence model of PHOENICS was selected as a proper turbulence model. This model allows for both laminar and turbulent flow conditions to be considered. It computes a local Reynolds number in every computational cell and applies the local effective viscosity based on this number. The effective viscosity includes both laminar and turbulent components. This allows for accurate modeling of fluid flow conditions within the whole domain.

3. Model validation

The CFD modeling of hydrogen release and dispersion needs to be validated before it can be widely applied to industrial projects.

3.1 Comparison of simulation results with published data

A hydrogen release problem with a simple geometry was used for validation of the above CFD model. In particular, in this scenario (see Figure 1), the hydrogen leaked from the floor at the left end of a hallway with the dimension of 114 in × 29 in × 48 in (2.9m × 0.74 m ×1.22 m). At the right end of the hallway, there were a roof vent and a lower door vent for the gas ventilation. Four sensors were placed in the domain to record the local hydrogen concentration variations with time. The numerical and experimental results for this benchmark problem were described in [2]. Figure 1 shows a comparison of the numerical results corresponding to the experimental results reported in [2], obtained using FLUENT (www.fluent.com) and obtained by Stuart Energy using PHOENICS. The grid used was a coarse grid of 36 × 10 × 18. It can be seen that the two different CFD codes gave very similar results. Figure 2 shows the concentrations at the four sensors obtained in [2] from numerical simulations using FLUENT and from experiments (left) and those obtained by Stuart Energy using PHOENICS. The concentration differences between the two models are about 20% for sensors 1 and 2 and 10% for sensors 3 and 4. The differences may be attributed to differences in the turbulence models, grid sensitivity, and/or the settings of boundary conditions at the inlet and the outlets (two vents).

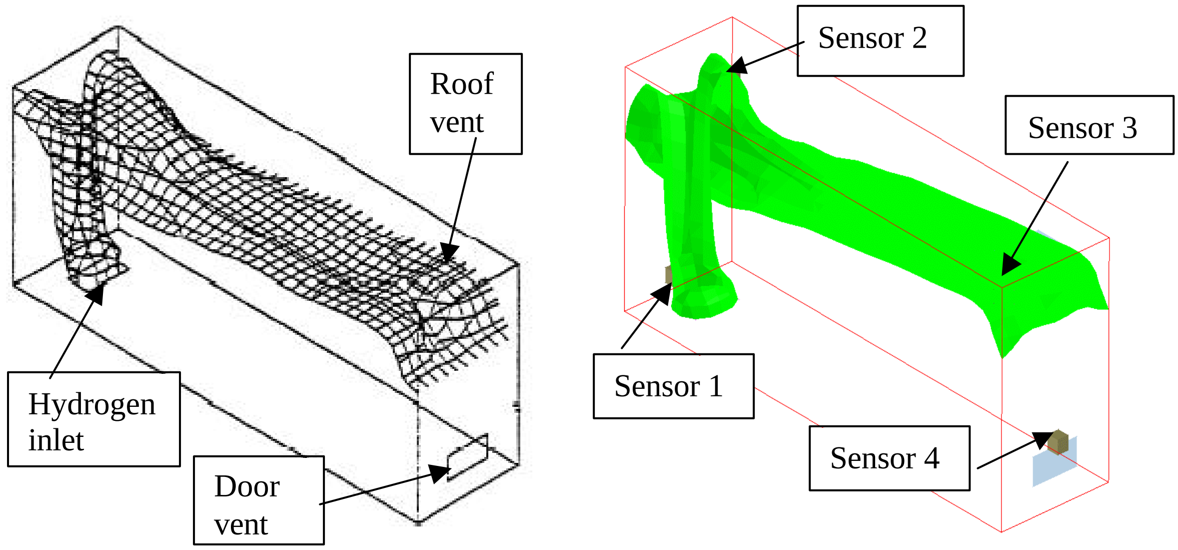

Figure 1. Comparison of concentration iso-surfaces for 2 SCFM hydrogen leak, 1 min elapsed and 3% concentration iso-surface. (Left: published data [2]; right: Stuart Energy's modeling).

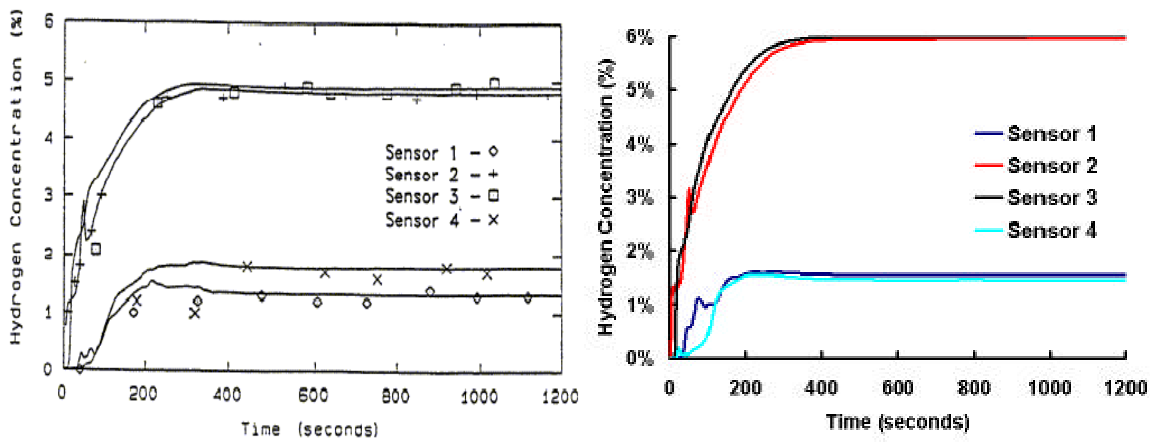

Figure 2. Comparison of concentrations at four sensors for 2 SCFM hydrogen leak and 20 minute duration. (Left: published data [2]; right: Stuart Energy's modeling).

3.2 Similarity theory

In order to validate the CFD modeling results, proper experimental data on hydrogen release and dispersion are required. For reasons of safety, helium was often used in validation experiments as an alternative for hydrogen [2]. However, helium and hydrogen differ in their thermodynamic and hydrodynamic properties, such as buoyancy, turbulence, diffusion and density, as can be clearly seen from the following similarity theory analysis.

The flow characteristics of gas release and dispersion in air depend on the five important non-dimensional parameters: the Reynolds number (*Re*), the Schmidt number (*Sc*), the Mach number (*Ma*), the Richardson number (*Ri*) and the density ratio (k_r), which are defined as follows to represent the turbulence, diffusion, compressibility, buoyancy and density difference effects, respectively:

$$\mathrm{Re} = \frac{UL}{n}, \quad Sc = \frac{n}{D}, \quad Ma = \frac{U}{V}, \quad Ri = \frac{(r_{air} - r_{gas})gL}{r_{gas}U^2}, \quad k_r = \frac{r_0}{r_{gas}}. \tag{5}$$

Here *U* is the gas (hydrogen or helium) release velocity at the orifice; *L* is the orifice size; ? is the kinematic viscosity of the gas (1.05×10^{-4} m^2/s for hydrogen and 1.15×10^{-4} m^2/s for helium); *D* is the diffusion coefficient of the gas in the air (6.1×10^{-5} m^2/s for hydrogen and 5.7×10^{-5} m^2/s for helium); r_{air} is the reference density, i.e. the air density, which is 1.209 kg/m^3 (at 1 atm and 20ºC); *V* is the sonic speed, which is $V_{H_2} = \sqrt{k_{H_2}R_{H_2}T} = 1305.61$ m/s for hydrogen and $V_{He} = \sqrt{k_{He}R_{He}T} = 1005.35$ m/s for helium; k_r is a key parameter characterizing the variable gas mixture density: $r = r_{air}(1+(k_r-1)C)^{-1}$ or $r = r_{air}(1+(k_r^{-1}-1)a)$. These parameters are calculated at the standard pressure and temperature: P=1.01×10^5Pa and T=293ºK.

The ratios of the Reynolds, Schmidt, Mach and Richardson numbers and the density ratios for the two gases are defined below to estimate the distortions between the flows of two gases:

$$a_{\mathrm{Re}} = \frac{\mathrm{Re}_{He}}{\mathrm{Re}_{H_2}} = 0.91, \quad a_{Sc} = \frac{Sc_{He}}{Sc_{H_2}} = 1.17, \quad a_{Ma} = \frac{Ma_{He}}{Ma_{H_2}} = 1.30, \quad a_{Ri} = \frac{Ri_{He}}{Ri_{H_2}} = 0.47, \quad a_{k_r} = \frac{k_{r,He}}{k_{r,H_2}} = 0.50. \tag{6}$$

The largest distortion of –53% is predicted for the Richardson number as (a_{Ri} -1) *100%= –53%. The large distortions result in significant differences in hydrogen and helium release processes: helium is less "turbulent" and "buoyant" but more "compressible" than hydrogen. The hydrogen buoyancy and turbulence effects would be underestimated if helium were used for validation of hydrogen modeling. The choked release velocity would be smaller and, as a result, the compressibility would be overestimated as well. Therefore it would be an improper approach to select helium instead of hydrogen for the validation experiments. Hydrogen, though combustible, has to be used for the validation of CFD modeling of hydrogen releases and dispersion. Results on further validation will be reported in a separate paper.

4. Modeling Scenarios and Numerical Results

The CFD model described in section 2 was applied to the simulation of hydrogen releases and dispersion in H2BPS. Two scenarios were considered in the simulations: a horizontal fast release from a high-pressure line and a vertical fast release from a medium-pressure line. In the case of a valve failure or line breaking, hydrogen may escape into the room from the high-pressure line between the CFA and the storage room. The duration of this release is limited by two factors. As soon as a pressure transducer senses a drop in backpressure, the CFA will shut down thus stopping hydrogen production. On the other hand, there is a non-return valve that makes back flow of hydrogen from storage impossible. It was estimated that the leak orifice size is ¼” on the tubing installed at the corner of CFA and the pressure in the tubing is 393 Bar, causing 0.037 m^3/s (normal cubic meter per second), or 3.1 g/s of hydrogen release rate. It is conservatively assumed that the duration of this high-pressure release is 10 seconds. Within this time period a command from PLC will shut the CFA down thus eliminating the source of release from CFA. The worst-case scenario is that the exhaust fan and ventilation duct are both closed. The CFD model simulated the horizontal hydrogen release under 10-second transient conditions. A structured grid of 36×36×33 was used for the simulation of this scenario. Another release scenario considers the case where, for whatever reason, during providing power to the building by one of the ICEs, the ball valve on the hydrogen feed line (medium-pressure of 11 barg), connecting the ICE and the storage tank, catastrophically fails or the line itself breaks away, thus resulting in 142 CFM (0.067 m^3/s) of horizontal hydrogen leak into the generator room. Meanwhile, the exhaust fan and ventilation duct are open and the ICE with the failure feed line (marked by “leaking ICE” in figure 4) continues to suck 2,725 CFM (1.29 m^3/s) room air and disperses all exhaust gases produced in its engine to the outside atmosphere. It is assumed that the duration of this medium-pressure release is less than 10 seconds. Within this time, after the backpressure in the line drops to 0.7 barg, a command from PLC will shut off the line between the ICE and the storage thus eliminating the source of release. The CFD model conservatively simulated 20-second leak duration with a structured grid of 44×39×39 for the whole domain.

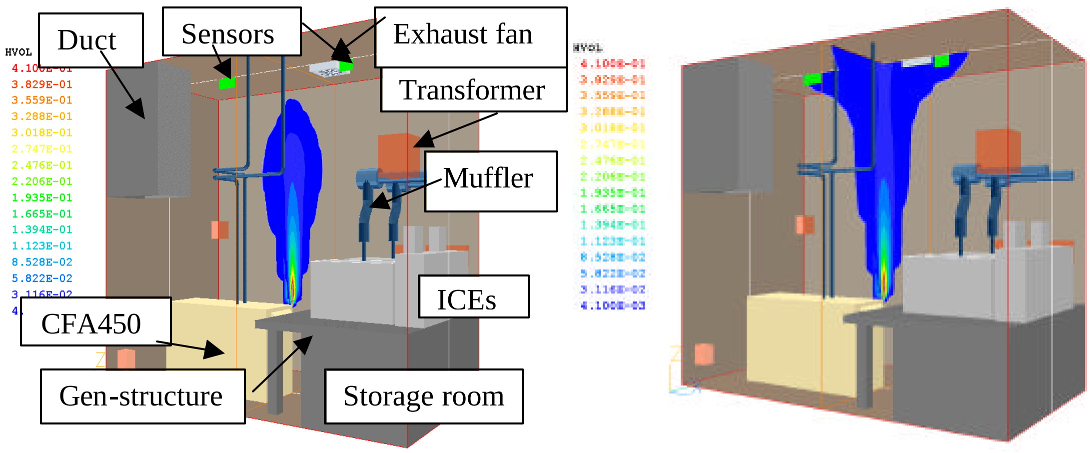

Figure 3. Hydrogen concentration distributions for vertical release of 0.0376 m^3/s from high-pressure pipe. (Left: at 5 sec.; right: at 10 sec.). A small portion of the room is occupied by the hydrogen cloud of more than 10% of LFL.

Figure 3 shows the hydrogen volumetric concentration distributions (0.41% to 4.1% vol.) for the vertical release from high-pressure pipe at 5 and 10 seconds. Within 10 seconds, the hydrogen cloud of 10% LFL (0.41% vol.) reaches the two sensors, which are marked by green color and located at the ceiling in the figure. The hydrogen cloud of 10% LFL occupies a small portion of top domain.

Figure 4 shows the hydrogen concentration distributions at the end of 5 and 20 seconds of horizontal release from one of the ICEs (right one). The hydrogen impinges onto the right wall of the generator room, resulting in relatively high concentrations in the region between the engine and the wall. 10% LFL (0.41% vol.) hydrogen cloud diffuses to top part of the room under the buoyancy, convection and diffusion effects.

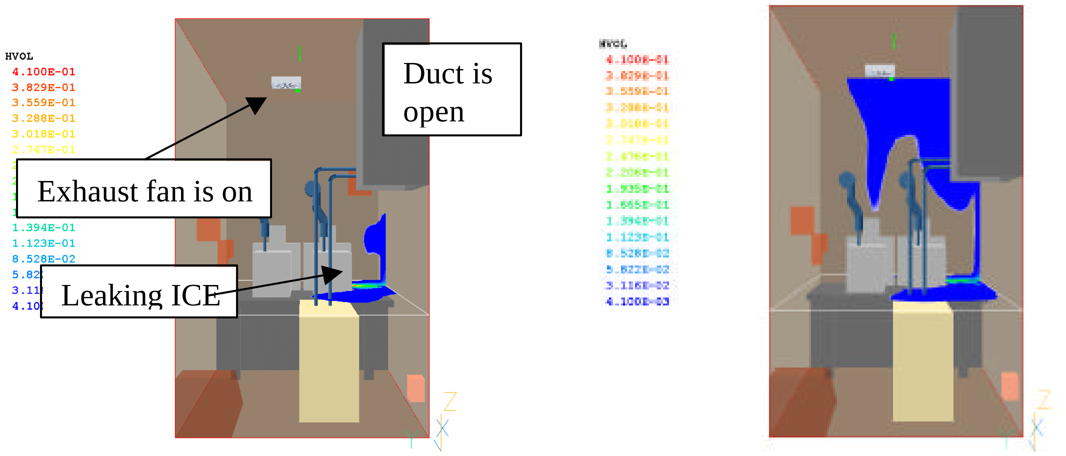

Figure 4. Hydrogen concentration distributions at horizontal and vertical planes that cross the leak orifice on the broken feed line for 0.067 m^3/s hydrogen leak. (Left: 5 sec; right: 20 sec). 10% LFL of hydrogen cloud reaches one sensor but it cannot reach the other within 20 seconds.

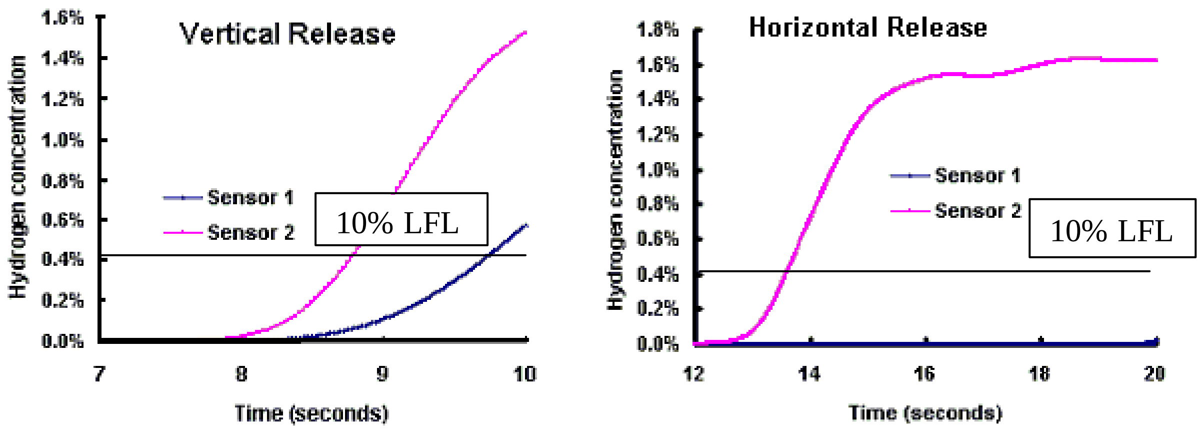

Figure 5. Hydrogen concentrations predicted at two sensors located on the ceiling. 10% LFL hydrogen cloud can be detected during the leak with current sensor installation.

Figure 5 shows the hydrogen volume fractions predicted at the locations of the two sensors for the two scenarios. It is seen that the two sensors are capable of detecting 10% LFL cloud (0.41%) separately at 8.8 and 9.7 seconds for the high-pressure vertical leak, but only one sensor which is closer to the leak orifice can detect the same concentration cloud within 20 seconds for the medium-pressure horizontal release. The numerical simulation confirms that the current sensor installation can promptly report the potential catastrophic hydrogen leak under the above scenarios and the explosion risks can be greatly reduced by the alarming systems. However, the fact that 10% LFL hydrogen cloud cannot reach one sensor during the horizontal release indicates that the sensor location can be further optimized and more sensors are required for the systems.

5. Conclusion

In this paper, a CFD model of hydrogen release and dispersion was described and validated through comparing the numerical results for a simple geometry with the published numerical and experimental data. Similarity of helium and hydrogen releases was also studied as -further validation of the model. The scaling analysis showed that similarity distortion in buoyancy, turbulence and compressibility of the two gases requires that validation experiments be performed using hydrogen. Finally, the CFD model was applied to HES for the prediction of hydrogen concentrations produced during some typical catastrophic releases. The numerical results allowed for evaluating the hydrogen risks and sensor efficiency in the HES. The HES, under the CFD modeling evaluation, has proven to be a safe and well-ventilated energy backup power station. CFD modeling results further demonstrated the advantages of using the gas release CFD models to assess the hydrogen risks in the HES room, as well as to facilitate obtaining further necessary approvals for Alpha H2BPS facility.

6. Acknowledgements

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7. References

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