CENTER FOR TRANSPORTATION INFRASTRUCTURE AND SAFETY

Safety Risks of Hydrogen Fuel for Applications in Transportation Vehicles

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16. Abstract

Combustion of hydrocarbon fuels in many practical applications produces pollutants that are harmful to human health and environment. Hydrogen fuel is considered to be a potential answer to the clean energy demands, especially with the advances in fuel cells and hydrogen powered internal combustion engines. The transition from fossil to hydrogen fuel involves many challenges that must be overcome for a widespread hydrogen economy. Safety is a critical issue during the design and operation of vehicles and storage tanks involving hydrogen, whose properties are drastically different compared to the traditional fuels such as gasoline. Experimental study and theoretical analysis were performed to investigate the flammability of hydrogen-air mixtures and its dependence on various parameters. To understand the transient behavior of hydrogen mixing and associated flammability limits in air during an accidental release, computational tools were used. The numerical simulations display the spatial and temporal distributions of hydrogen and the complex flow patterns demonstrate the fast formation of flammable zones with implications in the safe and efficient use of hydrogen in various applications. This study is essential to support the fire safety and prevention guidelines. Results obtained in this work are expected to be utilized for developing the necessary fire safety codes and standards for hydrogen-powered transportation vehicles and for the prevention and safe handling of hydrogen fires and detonations.

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Abstract

Combustion of hydrocarbon fuels in many practical applications produces pollutants that are harmful to human health and environment. Hydrogen fuel is considered to be a potential answer to the clean energy demands, especially with the advances in fuel cells and hydrogen powered internal combustion engines. The transition from fossil to hydrogen fuel involves many challenges that must be overcome for a widespread hydrogen economy. Safety is a critical issue during the design and operation of vehicles and storage tanks involving hydrogen, whose properties are drastically different compared to the traditional fuels such as gasoline. Experimental study and theoretical analysis were performed to investigate the flammability of hydrogen-air mixtures and its dependence on various parameters. To understand the transient behavior of hydrogen mixing and associated flammability limits in air during an accidental release, computational tools were used. The numerical simulations display the spatial and temporal distributions of hydrogen and the complex flow patterns demonstrate the fast formation of flammable zones with implications in the safe and efficient use of hydrogen in various applications. This study is essential to support the fire safety and prevention guidelines. Results obtained in this work are expected to be utilized for developing the necessary fire safety codes and standards for hydrogen-powered transportation vehicles and for the prevention and safe handling of hydrogen fires and detonations.

Keywords: Hydrogen safety; Flammability limits; Hydrogen dispersion

Introduction and Motivation

With the intensified energy and environmental concerns, hydrogen is considered to be one of the viable solutions to the increasing demands of clean and renewable energy. It might also enable fossil fuel importing economies to become leading exporters of hydrogen. Widespread public use and acceptance of hydrogen energy requires safety issues to be fully addressed by developing proper codes and standards that are critical for the design and operation of hydrogen-powered transportation and stationary systems. Fire safety of hydrogen applications is generally provided by experience from other traditional fuels whose properties are drastically different (e.g., density, mass diffusivity, flammability, detonability, flame visibility) from those of hydrogen. Established set of codes and standards for hydrogen are mainly based on large hydrogen industrial facilities. It is therefore essential to understand the properties of hydrogen, establish the safety codes and standards, and provide educational and training programs for an effective transition to hydrogen technologies.

As the hydrogen concentration decays in surrounding air during an unintended release, there is an envelope (approximately 4% and 75% by volume) beyond which the hydrogen-air mixture can no longer be ignited. These lowest and highest concentrations below and above which flame propagation cannot be sustained are called lower and higher flammability limits. Hydrogen flammability limits and their implications on fire safety and prevention are important in many applications such as hydrogen-powered transportation vehicles, hydrogen fueling stations, storage facilities, pipelines and other supplementary infrastructure. Buoyancy-driven diffusion of hydrogen in enclosures is also of interest in such applications because hydrogen gas can disperse very quickly with its lowest molecular weight. These properties can be used to avoid the formation of flammable mixtures after accidental hydrogen releases, and prevent further development towards hazardous concentrations. Based on properties alone, hydrogen poses an increased risk primarily due to increased probability of ignition, but the increased buoyancy effects, which are relatively difficult to assess, might change this probability depending on the actual physical condition.

Research Activities

Initially, a simple yet effective experiment was designed, constructed and set up in the Combustion Diagnostics Labs to observe the lower flammability limit (LFL) of hydrogen in air. Because the flammability limits depend not only on physiochemical properties of the fuel-air mixture but also heat loses from the system, the results are apparatus dependent. Several improvements and considerations were taken into account during these experiments. Efforts were made to find the LFL that would be obtained in free space, including: reducing the conductive-convective wall losses, making it less dependent on the direction of propagation of flame, i.e. the effect of buoyant convection and making it less dependent on diffusion mixing and flow gradient effects. The hydrogen LFL was found to be 5% by volume, which is close to the generally accepted value of around 4% in the literature. The difference was mainly attributed to the preferential diffusion of hydrogen in different experimental set-ups. This is because hydrogen has much less density than air and has high diffusion coefficient. Numerical simulation tools (explained later in the text) were used to understand this effect in detail.

A unifying semi-empirical model was developed based on the burning velocity of hydrogen-air mixtures to explain the various experimental results on LFL of hydrogen, including the present measurements. Dependence on the size of the combustion vessel, direction of flame propagation and heat losses due to conduction and convection was included in the model. The results predicted were compared with values reported in literature for different configurations and directions of flame propagation. The model was able to predict the trends relative to the experimental values well. This allowed estimates of the minimum recommended tube dimensions that would give lower flammability limit with negligible heat losses for different directions of flame propagation. The model will be an instrumental tool to predict the LFL of hydrogen in practical configurations such as the fire risks of accidental hydrogen leaks from high-pressure storage cylinders in transportation vehicles.

From literature survey it was found that hydrogen dispersion in a confined area is one of the most dangerous scenarios. However, there are few past investigations on the transient behavior during the process of mixing of hydrogen at short times. There is also a need to define a benchmark problem for simulating more complicated and practical hydrogen release scenarios with complex geometries. Exploration of the details of the temporal and spatial distributions of hydrogen in air and the resulting flammability zones has implications in the safe practices for hydrogen delivery to fuel cells as well as the ventilation of hydrogen accidental leakage in closed and partially closed environments (e.g., parking garage, road tunnel, fuel cell).

In the present work, different cases representing fundamental dispersion and leak phenomena are investigated within a vertical cylinder of 1 m height and 0.5 m diameter. Since the accurate predictions of formation and decay of flammable zones are difficult with experiments and theoretical hand calculations, advanced CFD tools are used here. These computations also provide deeper insight into the detailed hydrogen behavior with time. The computational parameters are varied so that the flow conditions are controlled by either buoyancy or molecular diffusion or jet momentum. Various cases that were considered are:

(i) Hydrogen is initially concentrated in the lower 10% volume of the cylinder with the remaining upper portion being air. At time t = 0 s, the hydrogen is released to allow mixing with the overlaying air in the absence of a momentum-forced jet. Cases with different top conditions are studied: (a) the top of the cylinder is completely open to the outside atmosphere, (b) the top of the cylinder has a circular opening of 0.25 m diameter (half the diameter of the cylinder) at the center, and (c) the top of the cylinder is completely closed. These cases are considered to understand the similarities and differences regarding the mixing processes of hydrogen/air and the corresponding flammable zones in closed, partially open, and open geometries.

Hydrogen mole fraction contours for the open cylinder top (case (a)) are shown in Fig. 1 at different time steps. Since hydrogen has high diffusion coefficient in air and very low density compared to air, it was found that hydrogen rapidly moves upward with the development of temporal and spatial concentration distributions within the unit-length vertical cylinder. With the commencement of mass transfer, the flammable mixtures begin to form depending on axial and radial locations at a certain time. The mixing process between these two gases with substantially different densities takes place by the combined effects of buoyancy and diffusion in the flow. The hydrogen concentration distribution depends on the convective mass transfer driven by buoyancy and molecular diffusion driven by local concentration gradients. At very short times (e.g. t = 0.1 s), hydrogen starts to disperse due to the local concentration difference where the distribution stays almost one dimensional in the axial direction. The buoyant force evidently assumes the predominant role after this initial time. As time progresses, hydrogen rapidly moves up, and its concentration decays from the initial high value forming a distribution that strongly depends on radial and axial positions across the cylinder. At these later times, the formation of small local pockets of higher hydrogen concentrations as well as the air entrainment to the lower cylinder portions can be seen in

Fig. 1. Hydrogen covers nearly all the cylinder volume as it reaches the cylinder top at about $t = 5$ s. Such a short time for the hydrogen to begin escaping from the unit-length vessel is associated with the strong buoyancy effects driven by the large differential between the molecular weights of hydrogen (2 kg/kmol) and air (29 kg/kmol). The time required for first emergence of hydrogen out of the cylinder into the open atmosphere is relevant to the estimation of evacuation times in larger size compartments.

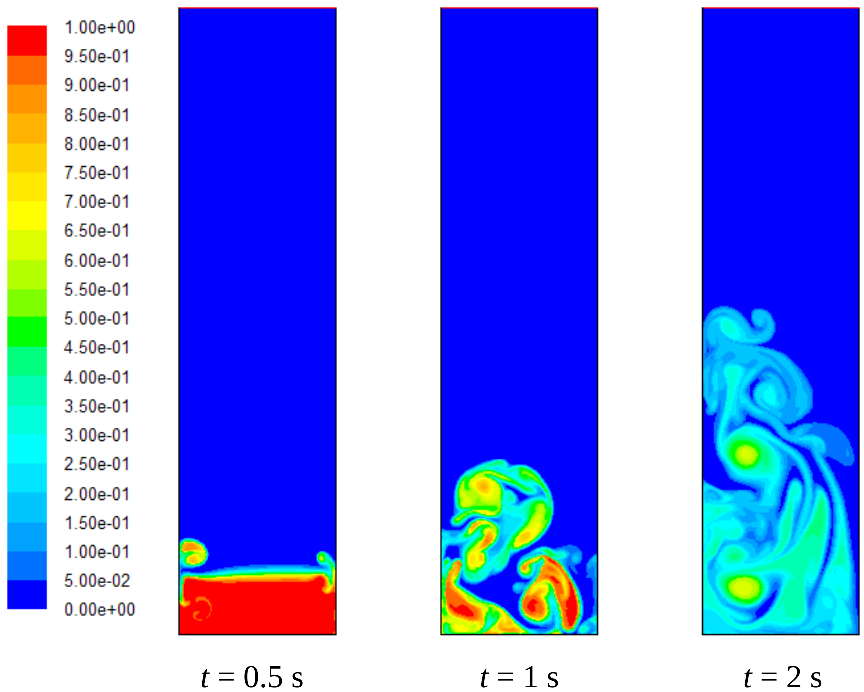


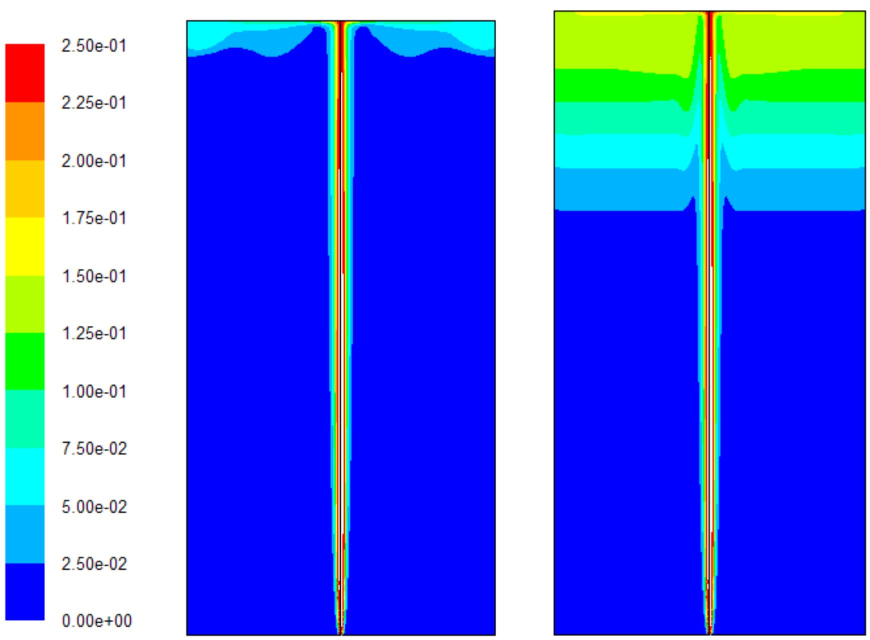
Figure 1. Hydrogen mole fraction contours for open top cylinder at different times

Similar to the open top case, complicated concentration contours dependent on both radial and axial position are again observed for cases with partially open top and closed top boundary condition. Despite a small amount of hydrogen release (10% by volume), flammable zones quickly cover a large portion of the container because of the relatively wide flammability limits. From a detection perspective, it was found to be better to install hydrogen sensors near the geometrical symmetry where hydrogen may rise faster. Naturally, extremely quick upward movement of hydrogen dictates the required response time from detection units.

(ii) Understanding the flammability envelope from a small-scale hydrogen leak and its transient dispersion properties is important for the safe use of hydrogen. Consequently, small continuous hydrogen leak from a hole of diameter 2 mm at the bottom center of the vertical cylinder is also considered. These conditions yield laminar flow at the jet exits with Reynolds numbers of 1000. Relative to the previous pure dispersion case, the jet momentum will force the hydrogen flow upwards and consequently influence the unsteady fluid dynamics. Hydrogen mole fraction contours at different time steps for the jet leak is shown in Fig. 2.

It was found that hydrogen concentration is confined to a very small region near the cylinder centerline until it hits the closed top with the jet momentum and buoyancy working together in the same direction of the flow. The first arrival of hydrogen at the cylinder top is less than 1 s, after which a stagnation point is formed that causes radial flow movement and concentration distribution. With no escape route in this enclosure, hydrogen then flows downwards and starts occupying the entire cross section of the cylinder at a very slow rate. While there are some variations in the radial direction, the concentration contours become nearly parallel with the emergence of uniform distributions. This indicates that the molecular diffusion takes over the mixing process once the jet momentum is lost to the top wall and the flow turns in the same direction of the gravitational force. These observations are again a result of the fact that hydrogen has a very low density compared to that of air.

These jet leak simulation results quantify the escape time for occupants in accidental releases of hydrogen within enclosures while there is a dependence of container volume, leak size and flow rate, and geometry. This work also shows that the occupants during a possible hydrogen accidental release in an enclosed area may have substantially more time, typically on the order of a minute (depends on the geometry), to escape underneath the gas accumulation near the ceiling. In contrast, a traditional fuel leak accumulates near the lower escape routes with a gas density similar to that of air and forms flammable mixtures typically within a few seconds and hence less time to escape.



t = 5 s t = 45 s

Figure 2. Hydrogen mole fraction contours at different times for a 2-mm-diameter leak at the cylinder bottom with Re = 1000

The above results have various safety implications in practical applications involving hydrogen transportation vehicles. The simple axisymmetric cylinder geometry with different hydrogen gas release scenarios considered here presents a basic model that may help explore more complicated features of real structures, especially the transient hydrogen behavior immediately after an accidental release. Some examples include hydrogen rises (and other relatively light gases) in air in open atmosphere, road tunnels, ventilated garages, and storage enclosures. This study also emphasizes the importance of proper ventilation and/or sufficient storage volume during the design of hydrogen systems.

Broader Impacts

In the present work, experimental study, theoretical analysis and computational simulations were performed to study the behavior of hydrogen mixing and the associated flammability limits in air during an accidental release. Results obtained in this project are to be ultimately utilized to develop necessary fire safety codes and standards for hydrogen-powered transportation vehicles and develop tools to help establish safety risks of hydrogen systems where there is a lack of history of actual use.

Relationship to other Research/Projects

The project is directly related to the recent efforts at Missouri S&T to establish a Hydrogen Center in order to pursue a broad research, training, and education agenda for the development of a rural hydrogen transportation test bed that will demonstrate, evaluate and promote hydrogen-based technologies in a real-world environment. In addition, currently hydrogen combustion in engines is being investigated using industry standard state-of-the-art engine simulation software GT-POWER. Internal combustion engines fueled by hydrogen have the potential for higher power and efficiency with lower emissions when compared to gasoline engines. Hydrogen engines also act as a transitional technology in hybrid vehicles during the development of a hydrogen economy. Advanced engine simulations provide cost-effective technical tools that considerably shorten the development time from conceptual ideas to actual products. Such tools are especially important for alternative fueled engines which are in the initial stages of development and commercialization.