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Hydrogen Flammability Limits and Implications on Fire Safety of Transportation Vehicles

by

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at Missouri University of Science & Technology**

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16. Abstract The recent establishment of the National University Transportation Center at MST under the "Safe, Accountable, Flexible, Efficient Transportation Equity Act: A Legacy for Users," expands the research and education activities to include alternative transportation fuels and other issues that are at the forefront of society and the national agenda. MST in partnership with MTI will establish a rural hydrogen transportation test bed for developing, demonstrating, evaluating, and promoting hydrogen-based technologies in a real-world environment. The State of Missouri is ideally suited to develop and demonstrate the proper operation of hydrogen highways in a rural setting, which represents over 25 percent of the nation's transportation needs and which is not well-represented in the current major national projects. A holistic approach will be taken to address not just the technology but also public perception, permitting, safety standards, and education and training. A key partner already engaged is the NASFM, who regards this project as an "excellent candidate for the model approach to introducing hydrogen to communities." The tasks identified in five areas, viz., Infrastructure Development and Deployment, High-Pressure Composite Cylinders, Inspection and Monitoring, Statistically Validated Codes and Standards, and Safety, constitute a comprehensive research, development and demonstration program to address some of the challenges described in the U.S. Department of Transportation Hydrogen Roadmap 2005.				
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Project Objective

The primary objective of this project was to investigate the flammability of hydrogen-air mixtures and its dependence on various experimental parameters by designing and constructing a test apparatus for the accurate measurement of flame propagation as well as to predict various properties of hydrogen fuel mixtures by computational modeling.

Introduction and Motivation

Hydrogen is an alternative fuel that is considered to be one of the viable solutions to the increasing demands of clean and secure energy. The transition from fossil fuels to such new technologies involves many challenges that must be overcome for widespread public use and acceptance. Safety issues need to be fully addressed by developing proper codes and standards that are critical for the design and operation of hydrogen-powered transportation vehicles. Fire safety of hydrogen applications is generally provided by experience from other traditional fuels whose properties are drastically different from those of hydrogen. Established set of codes and standards for hydrogen are mainly based on large hydrogen industrial facilities. It is therefore important to understand the properties of hydrogen, establish the safety codes and standards, and provide educational and training programs for the widespread use of hydrogen technologies.

Hydrogen has properties that are drastically different from traditional fuels. Key concerns are its low ignition energy, low luminosity, high flame speed, and wide flammability range. System and component design should accommodate the above special characteristics of hydrogen. The development of hydrogen-powered transportation vehicles will require safety guidelines for designing fueling stations, storage facilities, pipelines, and other supplementary infrastructure. Accidental hydrogen leaks from high-pressure storage units can lead to hazardous conditions because momentum-dominated large turbulent jet flames pose significant safety risks that need to be assessed. Design criteria for refueling stations requires the necessary distances between storage units and other materials/public places which can be determined by utilizing length, shape, and radiation heat of an ignited hydrogen plume.

As the hydrogen concentration decays in surrounding air during an unintended release, there is an envelope beyond which the hydrogen-air mixture can no longer be ignited. This lowest

concentration below which flame propagation cannot be sustained is called lower flammability limit (LFL). There is a great interest in hydrogen flammability limits and its implications on fire safety and prevention in many applications including hydrogen-powered transportation vehicles. Diffusion of hydrogen in enclosures is also of interest in such applications because hydrogen gas can disperse very quickly with its lowest molecular weight.

Research Activities

A Ph.D. student, Shravan Vudumu, was recruited to work on this project. He had an excellent experimental and computational background to study the various aspects of hydrogen fuel.

A complete literature survey was first conducted on hydrogen flammability limits. It was identified that the reported values for hydrogen lower flammability limit substantially varied from 4% to 9.5% by volume in air, depending on the experimental configuration employed. The general experimental methodology to determine the flammability characteristics of various combustible gases is usually based on the observation whether or not a flame ignited propagates the entire length of a tube. Because the flammability limits depend not only on physiochemical properties of the fuel-air mixture but also heat losses from the system, the results are apparatus dependent.

Following the previous work, a simple yet effective experiment, as illustrated in Figure 1, was designed, constructed, and set up in the Combustion Diagnostics Labs to observe the lower flammability limit of hydrogen in air. It involved a high-pressure hydrogen and a air gas cylinder that supplied their mixtures into a glass cylinder with calibrated mass flow meters. LAB VIEW data acquisition software was used to control the amount of hydrogen sent through the mass flow controllers in to the combustion tube. A custom-made ignition system was installed in the glass cylinder to provide a strong spark. If the mixture has sufficient hydrogen (above LFL), a flame can be observed that punctures the plastic top.



Figure 1. Experimental setup

Several improvements and considerations were taken into account during these experiments. Efforts were made to find the lower flammability limit that would be obtained in free space, including:

1. reducing the conductive-convective wall losses,
2. making it less dependent on the direction of propagation of flame, i.e. the effect of buoyant convection,
3. reducing radiation heat loss, and
4. making it less dependent on diffusion mixing and flow gradient effects.

The hydrogen LFL was found to be 5%, 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. The effect of the ignition energy and ignition gap distance was also found to affect LFL. Effect of various test factors, such as the shape and size of the combustion vessel, the direction of flame propagation, heat losses, and mixing level were also considered.

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. As can be seen in Figure 2, 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.

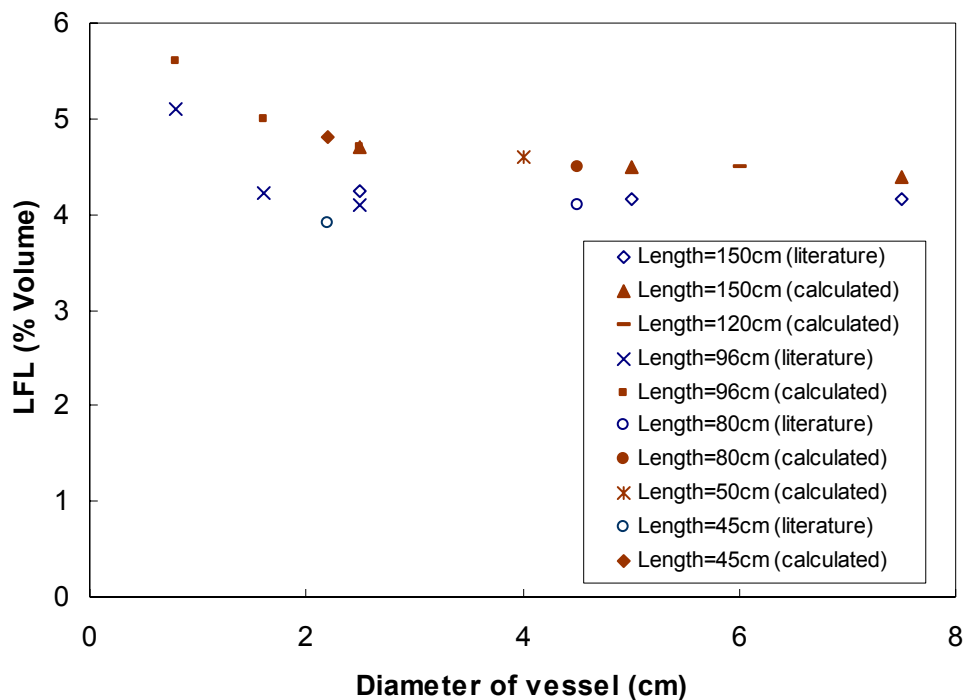


Figure 2. Measured and predicted LFL vs. vessel diameter for different lengths

In addition to the above experimental research activities, a transient diffusion-buoyancy computational model was adopted using the FLUENT software in order to account for fast diffusion of hydrogen. As well known, hydrogen has a high diffusion coefficient and a low density compared to the air and other hydrocarbon fuels. Computational fluid dynamics (CFD)

provides convenient tools to predict hydrogen behavior in practical situations, e.g. formation of flammable concentrations during an accidental leakage in hydrogen fueling stations or vehicles.

The first CFD application of FLUENT (Version 6.3) was related to the hydrogen dispersion in a vertical cylinder, similar to the present combustion chamber used in the LFL experiments. The governing equations of conservations of mass, momentum and energy were considered under unsteady axisymmetric conditions. Laminar non-reacting transport equations for two species (hydrogen and air) were solved. Second order implicit scheme was used to solve the unsteady flow equations for better accuracy. The governing equations were solved sequentially (i.e., segregated from one another) using pressure-based solver suitable for low speed incompressible flows. Because the governing equations were non-linear and coupled, the solution loop must be carried out iteratively in order to obtain a converged numerical solution. Incompressible ideal gas mixing law was used to compute the mixture properties. Stationary, no-slip and constant wall temperature (300 K) boundary conditions were applied on the walls of the cylinder.

In order to accommodate the highly diffusive nature of hydrogen:

- (a) Very fine non-uniform mesh with a minimum and maximum grid size of 0.001 mm and 0.8 mm respectively was used. A grid independent study was performed to make the simulations independent of grid size.
- (b) A very small time step of 10^{-4} seconds was used. Forty iterations were performed at each time step for convergence to be achieved at every time step.
- (c) Absolute convergence criterion for continuity and energy equation residual was 10^{-5} and 10^{-6} respectively.

As displayed in Figure 3, the CFD model was applied to the configuration employed during the experiments to observe the variation of hydrogen concentration at different time intervals. These simulations are currently being extended to other geometries to explore safe practices for hydrogen delivery to fuel cell and for ventilation of hydrogen accidental leakage in closed environments such as a garage.

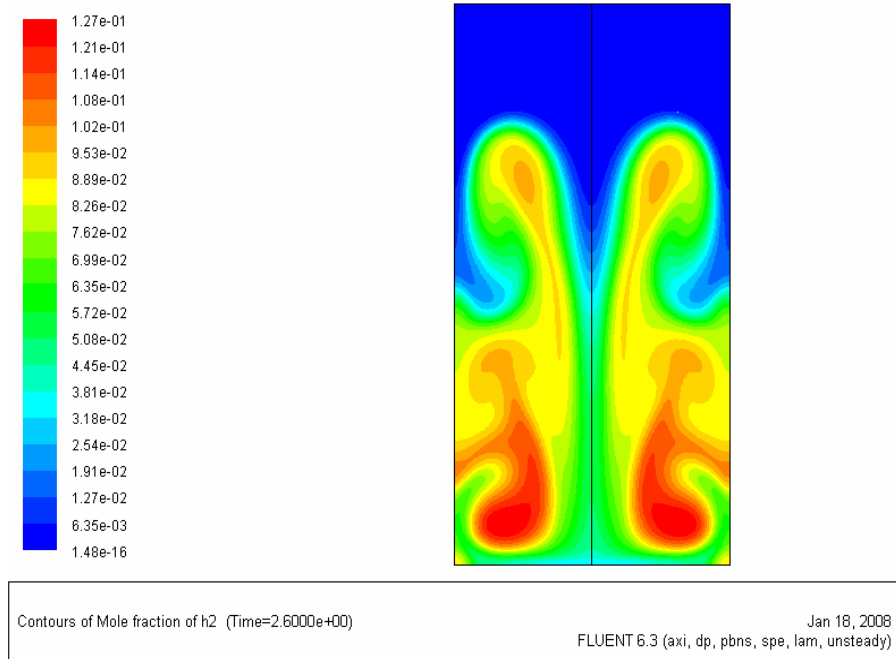


Figure 3. Computational simulation of hydrogen diffusion

Technology Transfer Activities

The findings of this research project were presented at the following meetings and conferences:

“Hydrogen Safety Training Material,” Hydrogen Executive Leadership Panel, Fall 2007 Meeting, Arlington, VA, November 6-7, 2007.

“Show Me the Road to Hydrogen,” 6th Fort Carson Community Sustainability Conference & Exposition, Colorado Springs, CO, October 30-31, 2007.

“A Rural Hydrogen Transportation Test Bed,” 2nd International Conference on Hydrogen Safety, San Sebastian, SPAIN, September 11-13, 2007.

Additionally, a paper entitled “Studies on Hydrogen Flammability Limits for Developing Safety Codes and Standards,” will be presented at the next Annual Hydrogen Conference of the

National Hydrogen Association in Sacramento, CA, March 30-April 4, 2008. An article is also planned to be submitted to the International Journal of Hydrogen Energy soon.

Broader Impacts

Results obtained in this project are to be ultimately utilized to develop necessary fire safety codes and standards for hydrogen-powered transportation vehicles. A preliminary database is being developed to help establish guidelines for the prevention and handling of hydrogen fires. Findings also have implications for the safe and efficient delivery of hydrogen fuel to fuel cells. The project therefore provides the much-needed fundamental data that are relevant to fuel cell bus operation where there is a lack of history of actual use.

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, A General Motors PACE project was recently obtained to utilize the GT-POWER software for complex internal combustion engine modeling. This software is an industry standard tool used by many leading vehicle manufacturers. This project allows the extension of simulation software to alternative fuels, including hydrogen, and consequently the exploration of hydrogen engine combustion with the consideration of safety issues and the necessary codes and standards. A proposal entitled “Show Me the Road to Hydrogen: A State and Local Government Outreach Program in Missouri,” was also submitted to the Department of Energy. This proposal will allow the education of state and local legislatures on hydrogen and fuel cells in order to stimulate market penetration of clean energy technologies.