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A computational fluid dynamics evaluation of unconfined hydrogen explosions in high pressure applications

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ABSTRACT

Over the last few decades, the demand for hydrogen has significantly grown. Its high-energy content and relatively small environmental effect make it an ideal energy source and chemical feedstock. However, the perceived high risk of hydrogen in the eyes of society is a key challenge that has to be addressed before any future widespread utilization of hydrogen can be achieved. In this study, the consequences of unconfined hydrogen releases are evaluated using a computational fluid dynamics simulation software, FLACS, to determine the potential to explode. In addition, the study includes the analysis of parameters that can promote hydrogen vapor cloud explosion, *e.g.*, initial pressure, time to ignition, and leak height position.

The results conclude that high-pressure hydrogen has the potential to build up a large vapor cloud and may explode even without confinement when the leak source is close to the ground. The highest overpressure produced in the simulation was 0.71 barg, which resulted from igniting a hydrogen gas cloud from a 207 bar hydrogen source leaking at 1 m height. The high overpressure suggests that hazard studies for hydrogen leaks near the ground should not assume a free flow jet release. This study also gives a recommended distance from a high-pressure hydrogen processing unit to nearby occupied buildings to use in conjunction with industrial spacing tables for fire hazards.

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Introduction

Hydrogen has been gaining popularity as a fuel and chemical feedstock over the last decades. There is a large interest in producing and consuming hydrogen in different industries. In 2017, the global production of hydrogen is estimated to be around 65 million tonnes; around 95% of which was consumed in ammonia and methanol productions and in the hydrodesulfurization process [5,33]. With the abundant discoveries of shale gas, a major monetization route involving the production of synthesis gas (syngas), which is composed primarily of hydrogen and carbon monoxide has emerged. Syngas can be used to produce a wide variety of chemicals such as ammonia, methanol, dimethyl ether, formaldehyde, acetic acid, and Fischer-Tropsch liquids [1,2,7,20,29,35]. Shale gas can also be aromatized to benzene and other products, with hydrogen being the main byproduct [36]. Furthermore, ethane and propane from shale gas are becoming the preferred feedstocks to produce ethylene and propylene with significant amounts of by-produced hydrogen. Such an emerging supply of surplus hydrogen is creating opportunities for integration opportunities within the same facilities or among adjacent facilities involved in industrial symbiosis [21,34].

Despite its versatile use, hydrogen production, transportation, and utilization involve many safety hazards and must be seriously taken into consideration. Hydrogen has a dense energy content, but with the tradeoff of a high probability of accidental fires and explosions. Hydrogen has a wide range of flammable concentration (4%–75% v/v) and a low ignition energy (1/10 of what is needed to ignite gasoline vapor), resulting in the highest rating on the flammability scale by the NFPA 704. Therefore, it is very important to study hydrogen safety in relation to its flammability and explosive characteristics.

More than half of all the reported hydrogen incidents in HIAD (Hydrogen Incident and Accident Database) from 1985 to 2012 involved an explosion, and 73% of all casualties had been linked with explosions ([26]). Industries have tried to mitigate the hydrogen explosion risk by placing hydrogen utilization and storage units in unconfined areas. It is generally accepted that a hydrogen release in a confined area will result in an explosion, but without any confinement, there is a general impression that hydrogen will not produce a flammable cloud of a significant size due to its light density and positive buoyancy. However, there have been at least 14 incidents involving hydrogen VCEs (Vapor Cloud Explosion) where hydrogen was ignited without any confinement, proving that this assumption is not reliable [39]. A hydrogen VCE incident in Polysar Petrochemical Complex in Sarnia, Canada underwent a deflagration to detonation transition (DDT) without any confinement and caused structural damages to buildings 900 m away from the ignition source [28].

Even with the current track record, the possibility of an unconfined hydrogen VCE in a facility is still a matter of debate and has been the subject of several research efforts. Dorofeev evaluated the hazard of hydrogen-air-steam explosion with focus on detonation onset and propagation conditions that can lead to an explosion [18]. Astbury and Hawksworth reviewed the postulated mechanisms for spontaneous ignition of hydrogen leaks [6]. Crowl and Jo analyzed the risks of hydrogen relative to gasoline and methane based on the physical properties of such fuels but without including the process of storage or release [14].

Field experiments on hydrogen explosions are not an economic nor a safe approach, as hydrogen is both dangerous and expensive to test in a safe environment. Computational Fluid Dynamics modeling is an alternative to accurately predict a chemical dispersion, fire, and explosion in a certain environment. There are other simplified prediction tools for hydrogen dispersion and explosions and assessment of safety distances for hydrogen explosions [18]. While easier and faster to use, those tools lack the ability to model the relevant physics and predict the effects of a certain incident. CFD-based risk assessment has been proven as a valuable and reliable method to evaluate hydrogen safety [31]. A number of hydrogen dispersions and explosions in various geometric conditions (confined and unconfined) has been simulated with CFD modeling and validated against experiments data [10,16,27,39,42] analyzed the hydrogen-air explosion that occurred in an ammonia plant in Norway, which resulted from hydrogen leakage [10].

This work focuses on validating the possibility of accidental hydrogen explosions in unconfined and uncongested area. The motivation behind this study has been to improve hydrogen safety knowledge and to develop recommendations for the industries on how to better prepare their facilities for prevention, mitigation and response for scenarios involving hydrogen explosions.

Problem statement

The main problem addressed in this study is the uncertainty of whether an accidental hydrogen release can explode without a confinement. The study was conducted by CFD modeling of hydrogen releases using a commercial CFD software FLACS (Flame Acceleration Simulator) to determine whether unconfined hydrogen VCE should be considered as credible events. In addition, analysis was conducted to study the process parameters that can promote the intensity of hydrogen VCE. Finally, the study provides recommendations on safety distances between a hydrogen facility unit and occupied buildings to minimize injury and property damage.

Methodology

This study presents numerical simulations of a hydrogen leak scenario in an unconfined and uncongested environment using FLACS v10.5. FLACS is a CFD modeling software that has been developed since 1980 to simulate atmospheric dispersion, fire, and explosion. FLACS solves compressible conservation equations on a 3D Cartesian grid using a finite volume method. The key advantage of this software is that it uses distributed porosity to represent geometry and therefore is able to simulate complicated geometries using a Cartesian grid while still maintaining reasonable simulation times.

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