Flame characteristics of ignited under-expanded cryogenic hydrogen jets

Ren, Z.X. and Wen, J.X
[1] Warwick FIRE, School of Engineering, University of Warwick, Coventry, CV4 7AL, UK,
jennifer.wen@warwick.ac.uk

ABSTRACT

The anticipated upscaling of hydrogen energy applications will involve the storage and transport of hydrogen in a cryogenic state. Understanding the potential hazard arising from small leaks in pressurized storage and transport systems is needed to assist safety analysis and development of mitigation measures. The current knowledge of the ignited pressurized cryogenic hydrogen jet flame is limited. Large eddy simulation (LES) with detailed hydrogen chemistry is applied for the reacting flow. The effects of ignition locations are considered and the initial development of the transient flame kernel from the ignition hot spots is analysed. The flame structures, namely side flames and envelop flames are observed in the study, which are due to the complex interactions between turbulence, fuel-air mixing at cryogenic temperature, and chemical reactions.

1 INTRODUCTION

Hydrogen is a carbon-free fuel for energy utilization with a high gravimetric energy density, but its volumetric energy density, especially under conditions of atmospheric temperature and pressure, is low. The volume of the hydrogen storage unit impedes the application of hydrogen. High pressures and/or low temperatures can be used to improve the volumetric energy density of hydrogen and the cryo-compression is a competitive technique for storage [1]. Understanding the potential accidents with the cryogenic release of hydrogen is fundamental to prevent loss. Accidentally leaked cryogenic hydrogen will form high-pressure under-expanded jets and even jet flames under the conditions of an external fire source. Delayed ignition may even cause a hydrogen explosion.

For the accidental leakage from small holes, the high-pressure liquid hydrogen is ejected through the nozzle to form an under-expanded jet. Under the influence of the complex wave system in the near field of the jet and the heating of the external environment, the low-temperature liquid undergoes atomization and phase change to form hydrogen, which mixes with the oxygen in the environment. And form a combustible mixture, under the influence of a certain external ignition source or heat source, a rapid chemical reaction occurs and forms a jet flame or local deflagration [2]. The low-temperature and high-pressure conditions of the liquid hydrogen jet significantly change the mass, momentum, and heat transfer law between the gas and liquid phases. Therefore, the hydrogen mass fraction, velocity, and temperature distribution in the far-field from the leakage have a big difference from those of the normal temperature and high-pressure hydrogen jet.

The experiment studies on cryogenic hydrogen jet flame were mainly carried from Sandia National Laboratory (SNL) and Karlsruhe Institute of Technology (KIT). Panda and Hecht[3] from SNL experimentally studied the ignition characteristics of a low temperature/normal temperature hydrogen jet with a total pressure of 0.2-0.6 MPa and a total temperature of 37-295K and obtained the dependence of the maximum ignition position on the hydrogen mass flow rate and temperature. Compared with normal temperature hydrogen Jet flow, the maximum ignition position of low-temperature hydrogen is longer, and the flame length is longer. Later, Hecht and Chowdhury cooperated to study the effect of rectangular nozzle aspect ratio on low-temperature hydrogen jet flame[4, 5]. They found that the nozzle aspect ratio had no obvious effect on the distribution of hydrogen concentration and flame length/width. Generally, their low-temperature hydrogen jet experiment has a lower pressure and a laminar jet flame, which is somewhat different from the actual high-pressure turbulent jet. Veser et al.[6] from KIT carried out experimental research on low-temperature hydrogen jets with a total temperature of 35K and 80K. The effects of total hydrogen pressure, nozzle diameter, and ignition position were considered. The experiment used probes and particle image velocimetry (PIV) to measure the concentration distribution of hydrogen. With the airflow speed, the flame propagation process is photographed through high-speed photography. The study found the correlation between the flame propagation direction and the local hydrogen concentration: when the hydrogen concentration is greater than 11%, the flame propagates toward the upstream and downstream of the jet at the same time; when the hydrogen concentration is less than 11%, the flame only propagates downstream or extinguishes. Afterwards, Friedrich et al.[7] conducted experimental studies on low-temperature hydrogen jets with a total temperature of 35-65K and a total pressure of 0.7-3.5MPa. The study found three flame propagation modes under the influence of different jet conditions and nozzle diameters: ignition, flame backfire to the nozzle, and stable jet flame; stable lift flame without backfire; short burning and then extinguishment. But they did not explain the relevant physical mechanism.

Due to the limitations of experimental equipment and measurement methods, numerical simulation has become an important technical method. However, the simulations are changing. Cirrone et al. [8-10] from Ulster University studied the low-temperature hydrogen jet flame experiment of SNL based on the numerical simulation of the notional nozzle model, and the results showed that the numerical model used can reasonably predict the changing trend of flame length and radiant heat flux.

Based on the above review, there is a lack of investigations on transient features of the formation of the flame kernel and the propagation of flames of the ignited releases, i.e., jet flame. Therefore, the present study aims to use the numerical simulation to predict the transient flame dynamics from a cryogenic jet and the effects of the ignition locations are considered.

2 MATHEMATICAL MODEL

Large eddy simulation (LES) of the unsteady ignited cryogenic hydrogen jet flame is conducted based on rhoReactingFOAM, which is a density-based compressible reacting flow solver with the frame of open-source computational fluid dynamics (CFD) code OpenFOAM. In LES all variables are decomposed into resolved and unresolved (subgrid) components by filtering reactive Navier–Stokes equations. The governing equations are solved for three conservative variables, specifically density, momentum density, and total energy density. A transport equation is also applied in order to consider mixing of multiple species. One-equation eddy-viscosity SGS model for compressible flows is used in which a transport equation is solved to resolve the Subgrid Scale (SGS) kinetic energy[11]. The eddy dissipation concept (EDC) model[12] is used for combustion and detailed hydrogen chemistry (9 species and 19 steps)[13] is applied. The finite volume discrete ordinates model (FVDOM) is employed to solve the radiative heat transfer equation (RTE). The weighted sum of the grey gas model is used to evaluate the absorption, emission coefficients.

A Finite Volume (FV) method is utilized to discretize the filtered partial governing equations into a set of resolvable linear equations. For discretization it is required to obtain fluxes of various flow variables at cell faces using the values at cell centres. The second-order Total Variation Diminishing (TVD) scheme and the Crank–Nicholson scheme are applied. The Courant–Friedrichs–Lewy (CFL) number is less than 0.5, corresponding to a physical time step at the order of 1×10^{-7} s.

3 BOUNDARY AND INITIAL CONDITIONS

Figure 1 shows the three-dimensional (3D) cylinder computational domain selected to analyse the ignited cryogenic hydrogen jet flame. The size of the diameter of the domain is set as 2 m and the height is 3 m based on pre-calculations of the hydrogen jet. The influence of boundaries on the evolution of the jet is checked so that no significant velocities were formed at the boundaries. The side, top, and bottom boundaries of the domain are set as open atmosphere, in which the boundary does not influence the flow across the domain. The hydrogen inlet is circular and located at the centre of the bottom plane (*x*-*y* plane, $z = 0$). The experiments were conducted with the DisCha facility at Karlsruhe Institute of Technology and were performed at cryogenic temperatures (80 K). According to experiment measurement[2], the total pressure is 200 bar, and the total temperature is 80 K. The nozzle diameter is 4 mm. Due to the high reservoir pressure of hydrogen; the throat of the nozzle can remain at higher than ambient pressure and, consequently, form an under-expanded jet from the nozzle. The calculations are made assuming isentropic expansion from storage to throat conditions. The notional nozzle model is applied[14] to estimate the flow conditions when the jet has expanded to ambient pressure. The hydrogen is injected from the bottom along the *z*-direction with a constant upward velocity. Initially, the domain is filled with stagnant air at T_a = 300 K and the ambient pressure is P_a = 1 atm. The grid spacing of 2 mm is applied in the simulation and the number of the grids is 20 million. This means that the eddy with the size above 2 mm is resolved and turbulence at the scales below 2 mm is assumed to be isotropic and homogeneous.

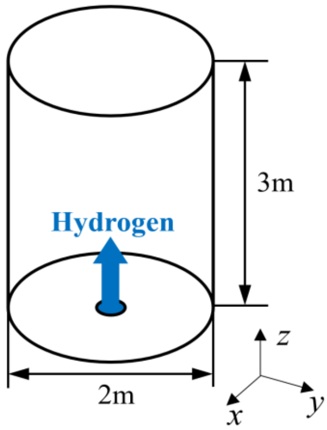


Figure 1. Schematic diagram of the computational domain.

The ignition sources (hot spot) are set with different streamwise locations, z_{ig}, along the centreline. The temperature of the hot spot is 2000 K, which is close to the ambient flame temperature of the stoichiometric mixture of hydrogen and air at normal conditions, and the volume is a cube with a side length of 2 cm. Three cases are applied with different z_{ig}, as shown in Table 1. The unignited jet, named UG, is also applied to make a compression.

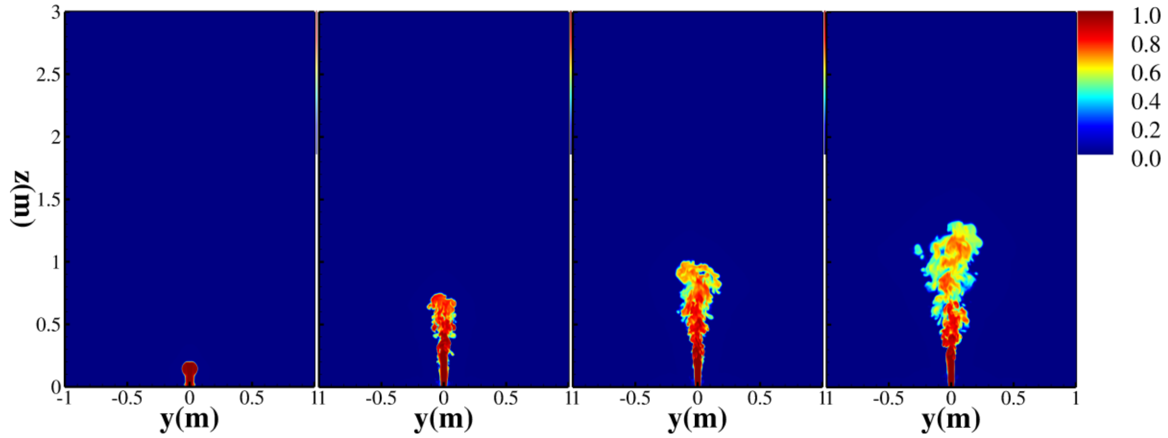
Table 1. Simulation cases.

Case #	UG	10IG	15IG	20IG
Ignition location (m), z_{ig}	/	1.0	1.5	2.0

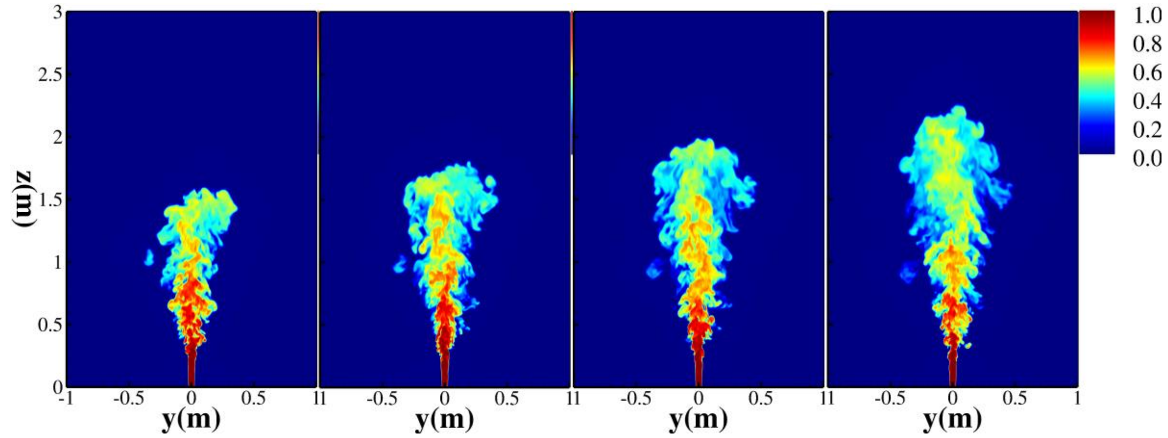
4 RESULTS AND DISCUSSION

4.1 Unignited jet

Figure 2 shows the evolution of the cryogenic hydrogen jet without the external hot spot for Case UG. The snapshots of the spatial distributions of hydrogen mole fraction are provided. At the time t = 1 ms, the hydrogen jet has penetrated into the ambient air and the jet tip has a regular round shape. With the evolution of the jet flow, it is found that the shape of the jet tip tends to be corrugated and the vortices are formed around the jet due to the shearing between the high-speed hydrogen flow and the ambient air. As shown by the snapshot at t = 10 ms, the mixing between hydrogen and surrounding air leads to the decrease of the hydrogen mole fraction at the jet tip. The hydrogen gas disperses towards the transverse directions. Due to the momentum transfer from the hydrogen jet to the ambient air, the penetration speed of the jet decreases continuously, as shown in Figure 2(b). Large-scale vortices entrained the air to mix with the hydrogen inside the jets and the reactive mixtures are formed in the far-field region from the nozzle, which is expected to lead to the flames with the suitable external hot spots.



(a)

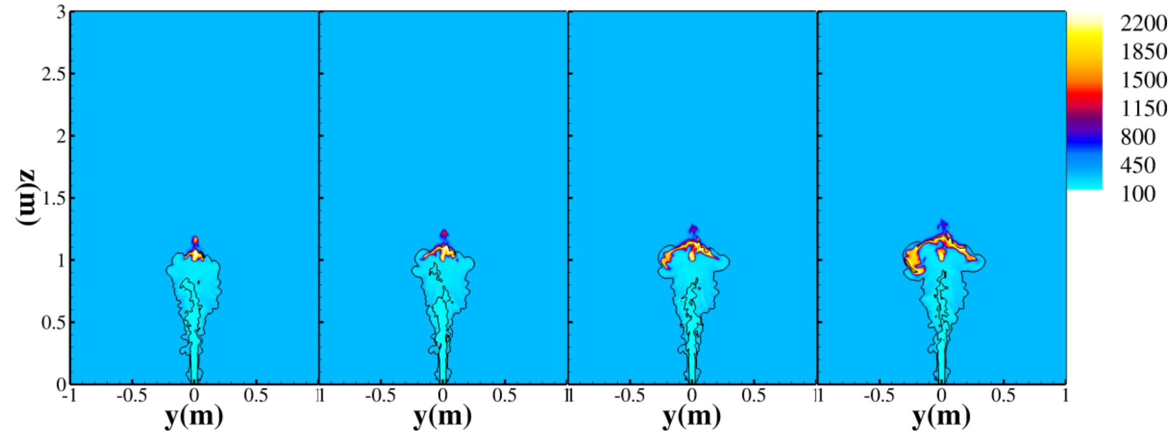


(b)

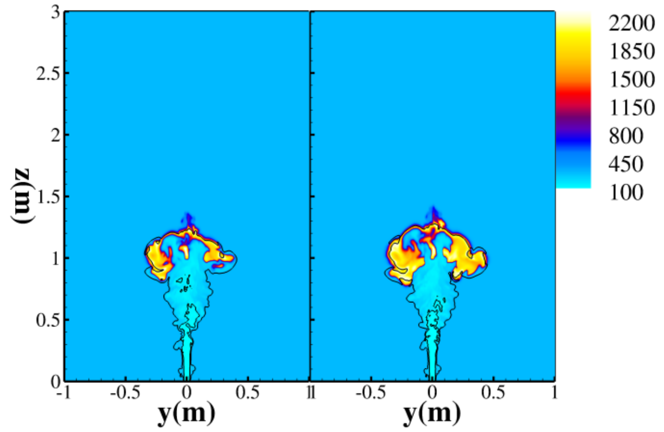
Figure 2. Instantaneous distributions of hydrogen mole fraction, Mol_{H2}, at *y-z* plane: (a) time from left to right: 1 ms, 5 ms, 10 ms, and 20 ms, (b) time from left to right: 30 ms, 40 ms, 50 ms, and 60 ms.

4.2 Near-range ignition

For Case 10IG with the ignition hot spot located at z_{ig} = 1.0 m, the instantaneous distributions of the temperature are shown in Figure 3. The regime enclosed by the black lines refers to the flammable area. It is found that as the hydrogen jet penetrates in the ambient air, the jet tip interacts with the hot spot at an early stage, as shown by the snapshot at time t = 12 ms. Spotted flame kernels are formed around the jet tip. The flame kernel then propagates outwards but cannot propagate towards the jet centre. It is mainly because the low temperature of the hydrogen impedes the chemical reaction on the jet tip. The flame propagates to the sides of the jet and then the flame area expands, as shown by the snapshots from 15 ms to 17 ms. This is because that the shearing on the sides of the jet promotes the mixing between hydrogen and air and also increases the temperature of the local hydrogen-air mixture from the heat transfer. Therefore, the side flame is formed from the near-range ignition.



(a)

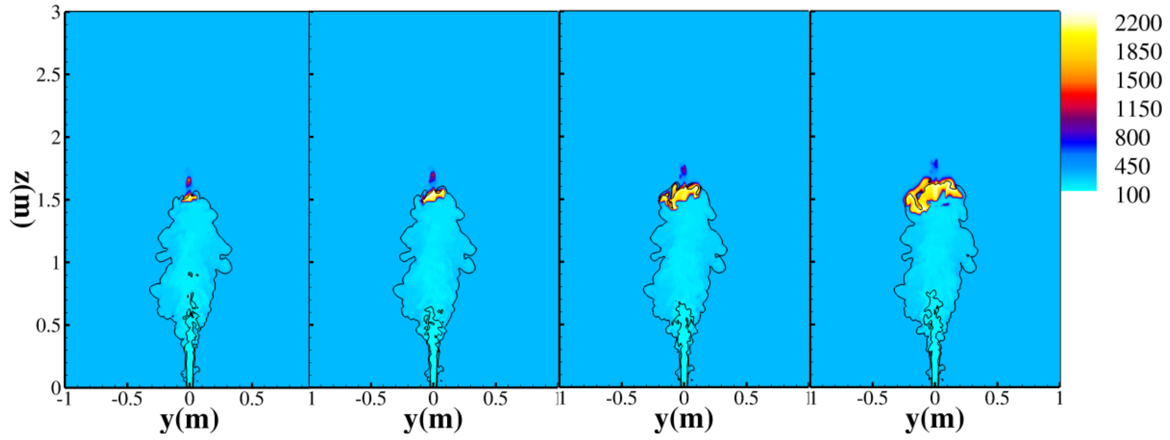


(b)

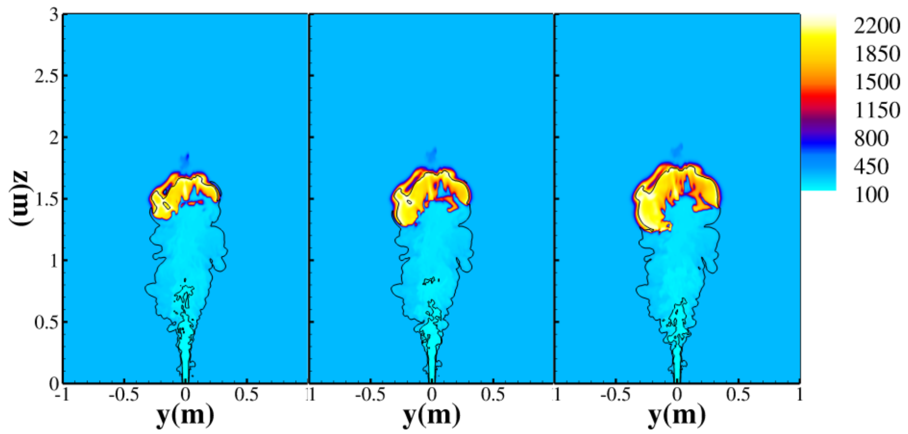
Figure 3. Development of flame kernel for the near-range ignition: (a) time from left to right: 12 ms, 13 ms, 14 ms, and 15 ms, (b) time from left to right: 16 ms and 17 ms. Here the contours refer to temperature (K) distribution at the *y*-*z* plane and the black iso-lines refer to the hydrogen explosion limit, Mol_{H2} = (0.040, 0.756).

4.3 Medium-range ignition

The ignition spot with the high temperature is set at z_{ig} = 1.5 m for Case 15IG and Figure 4 shows the formation and evolution of the flame kernel. The hydrogen jet interacts with the hot spot and induces a flame kernel, as shown by the snapshot at the time t = 25 ms. Compared with Case 10IG with the near-range ignition, the flame kernel not only propagates towards the jet centre but also approaches outwards to envelop the jet tip. For Case 15IG with downstream ignition, the temperature of the jet tip increases, and the mixing level of the hydrogen and air also increases, therefore promoting the chemical reaction around the jet tip and the flame propagates inside the jet. An envelope flame is formed to wrap the jet tip, as depicted by the flame structure at time t = 31 ms.



(a)



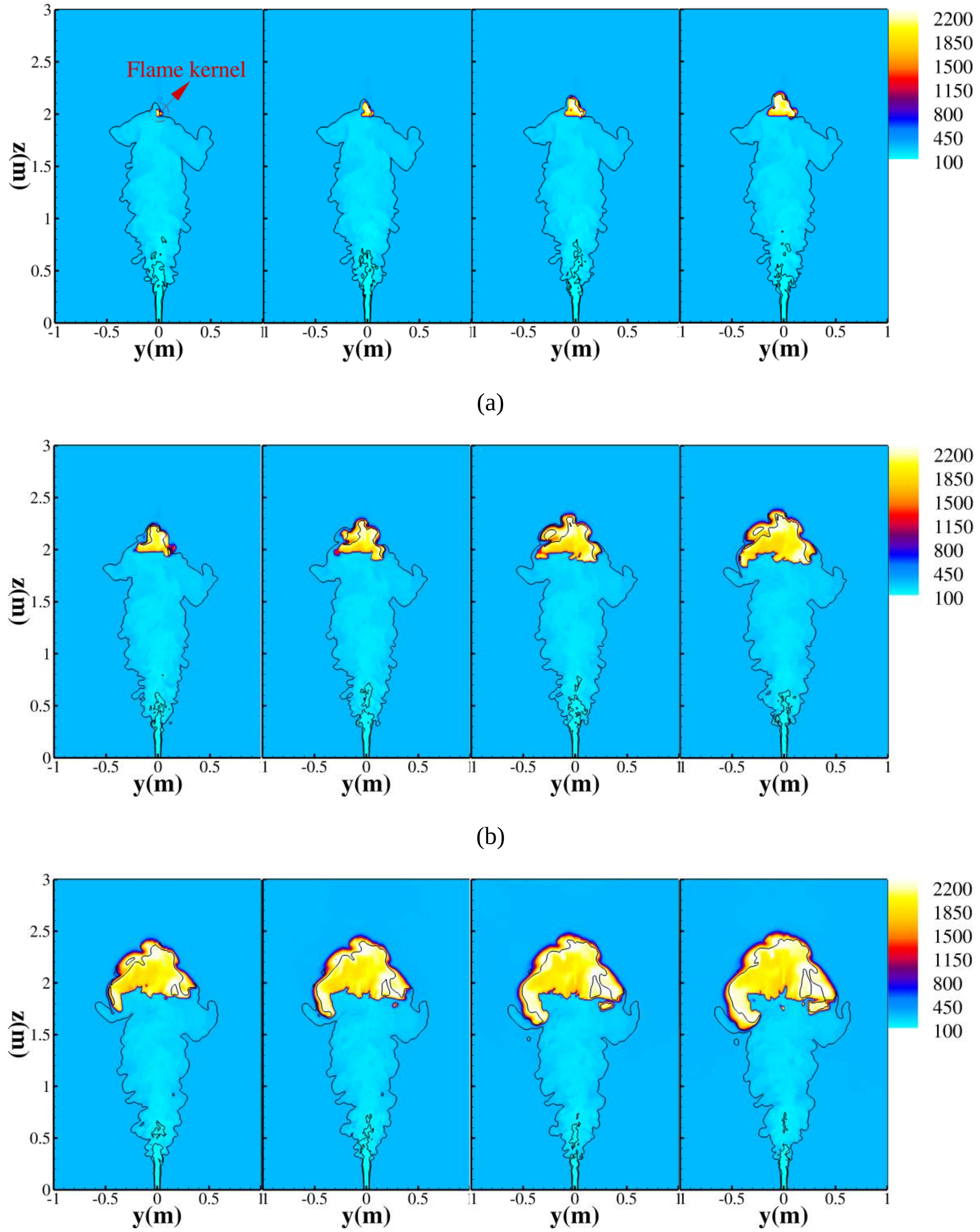
(b)

Figure 4. Development of flame kernel for the medium-range ignition: (a) time from left to right: 25 ms, 26 ms, 27 ms, and 28 ms, (b) time from left to right: 29 ms, 30 ms, and 31 ms. Here the contours refer to temperature (K) distribution at the *y*-*z* plane and the black iso-lines refer to the hydrogen explosion limit, Mol_{H2} = (0.040, 0.756).

4.4 Far-range ignition

For Case 20IG with the ignition hot spot located at z_{ig} = 2.0 m, the hydrogen and ambient oxygen are expected to form a premixed reactive mixture before interacting with the hot spot. After the reactive mixture disperses to interact with the hot spot, a flame kernel is formed at the tip of the jet, as shown by the snapshot at time t = 53 ms. Then the kernel propagates to burn the surrounding reactive mixture and the flame area increases continually, as shown by the figures from time 54 ms to 57 ms. Due to the inhomogeneous spatial distribution of the hydrogen, the flame surface tends to become corrugated. It is observed that the propagation of the flame accelerates from 57 ms to 60 ms. This is due to the fact that the wrinkle of the flame front increases the flame area. This, in turn, increases the hydrogen consumption rate and provides additional acceleration of the flame. Finally, the flame propagates to envelop the jet tip, as shown by the snapshot at time t = 64 ms, and the envelope flame structure is formed for the far-range ignition.

The initiation of the flame kernel induces a local high-pressure wave[2], as shown by the iso-surface of relative pressure equalling 5 kPa at time t = 56 ms in Figure 6. The pressure wave propagates outwards from the initial flame kernel.



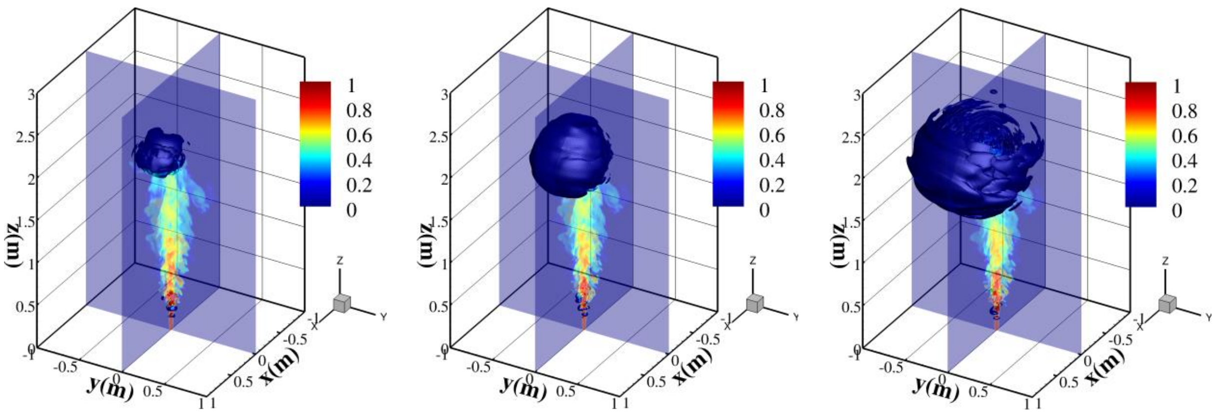
(a)

(b)

(c)

Figure 5. Development of flame kernel for the far-range ignition: (a) time from left to right: 53 ms, 54 ms, 55 ms, and 56 ms, (b) time from left to right: 57 ms, 58 ms, 59 ms, and 60 ms, (c) time from left to

right: 61 ms, 62 ms, 63 ms, and 64 ms. Here the contours refer to temperature (K) distribution at the *y*-*z* plane and the black iso-lines refer to the hydrogen explosion limit, Mol_{H2} = (0.040, 0.756).



(a) (b) (c)

Figure 6. Propagation of pressure wave for the far-range ignition: (a) t = 56 ms, (b) t = 57 ms, and (c) t = 58 ms. Here the contours refer to hydrogen mole fraction, Mol_{H2}, and the blue iso-surface indicates the relative pressure, $\Delta P = P\text{-}P_a$ = 5 kPa.

5 CONCLUSIONS

In the present study, a large eddy simulation with a detailed chemical reaction mechanism is applied for predicting the flame features of the ignited under-expanded cryogenic hydrogen jets. The compressible reacting flow solver, rhoReactingFOAM, with the frame of open-source computational fluid dynamics (CFD) code OpenFOAM is utilized. The influence of the ignition location on the flame dynamics is analysed. The results show that for the near-range ignition, the flame cannot propagate inside the cold jet and a side flame is formed. For the medium-range and far-range ignitions, an envelope flame around the jet is formed, which is attributed to the increase of the mixing condition and jet temperature in the downstream region. The unsteady flame dynamics are determined by the complex interactions among turbulence, fuel-air mixing at cryogenic temperature, and chemical reactions.

ACKNOWLEDGMENTS

The research is financially supported by the PRESLHY project, which has received funding from the Fuel Cells and Hydrogen 2 Joint Undertaking under the European Union's Horizon 2020 research and innovation program under grant agreement No. 779613. The authors are grateful to ARCHER2 for the computational support as a part of their funding to the UK Consortium on Turbulent Reacting Flows (www.ukctrf.com).

REFERENCES

1. Cirrone D M C, Makarov D, Molkov V. Thermal radiation from cryogenic hydrogen jet fires[J]. International Journal of Hydrogen Energy, 2019, 44(17): 8874-8885.

2. Friedrich A, Veser A, Necker G, Gerstner J, Kotchourko N. Ignited DisCha-Experiments[C]. 2nd PRESLHY Virtual Workshop on Experimental Outcomes, July 23, 2020.
3. Panda P P, Hecht E S. Ignition and flame characteristics of cryogenic hydrogen releases[J]. International Journal of Hydrogen Energy, 2017, 42(1): 775-785.
4. Hecht E S, Chowdhury B R. Characteristic of cryogenic hydrogen flames from high-aspect ratio nozzles[J]. International Journal of Hydrogen Energy, 2020.
5. Chowdhury B R, Hecht E S. Dispersion of cryogenic hydrogen through high-aspect ratio nozzles[J]. International Journal of Hydrogen Energy, 2020.
6. Veser A, Kuznetsov M, Fast G, et al. The structure and flame propagation regimes in turbulent hydrogen jets[J]. International Journal of Hydrogen Energy, 2011, 36(3): 2351-2359.
7. Friedrich A, Breitung W, Stern G, et al. Ignition and heat radiation of cryogenic hydrogen jets[J]. International Journal of Hydrogen Energy, 2012, 37(22): 17589-17598.
8. Cirrone D M C, Makarov D, Molkov V. Thermal radiation from cryogenic hydrogen jet fires[J]. International Journal of Hydrogen Energy, 2019, 44(17): 8874-8885.
9. Cirrone D, Makarov D V, Molkov V. Cryogenic hydrogen jets: flammable envelope size and hazard distances for jet fire[C]. International Conference on Hydrogen Safety. 2019.
10. Cirrone D, Makarov D V, Molkov V. Near field thermal dose of cryogenic hydrogen jet fires[C]. The Ninth International Seminar on Fire and Explosion Hazards. 2019: 1361-1367.
11. Yoshizawa A. Bridging between eddy-viscosity-type and second-order turbulence models through a two-scale turbulence theory[J]. Physical Review E, 1993, 48(1): 273.
12. Parente A, Malik M R, Contino F, et al. Extension of the Eddy Dissipation Concept for turbulence/chemistry interactions to MILD combustion[J]. Fuel, 2016, 163: 98-111.
13. Ó Conaire M, Curran H J, Simmie J M, et al. A comprehensive modeling study of hydrogen oxidation[J]. International journal of chemical kinetics, 2004, 36(11): 603-622.
14. Giannissi S G, Venetsanos A G, Hecht E S. Numerical predictions of cryogenic hydrogen vertical jets[J]. International Journal of Hydrogen Energy, 2020.