Lift-off and blow-out of under-expanded hydrogen jets: experiments versus simulations

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ABSTRACT

Turbulent non-premixed flame stability limits are very important for safety considerations, especially for design of thermally activated pressure relief devices (TPRD), e.g. to prevent flame blow-off and hydrogen accumulation in the enclosure. There is a body of research on parameters of lift-off and blow-out for turbulent non-premixed flames. Hydrogen safety engineering requires validated contemporary tools, such as CFD models, that can be used for the design of TPRD, which parameters will provide either the stabilisation of flame or its blow-off, including the effect of wind. The applied in this study CFD model is based on the eddy dissipation concept (EDC) sub-model for combustion, which incorporates a detailed chemistry mechanism with 37 chemical reactions, and the RNG k-epsilon sub-model for turbulence modelling. The model has been successfully applied to simulation of spontaneous ignition during the sudden release of hydrogen into the air, and the numerical study of indoor jet fire regimes. The notional nozzle theory for under-expanded jets is applied as a part of the CFD modelling approach. It is proved to be able to reproduce lift-off and blow-off phenomena that were observed in experiments, with reasonable computational consumption, i.e. CPU time of 6 hours on 64 cores. The model gives insights into the dynamics of the lift-off and blow-off phenomena. The simulations reproduced exactly experimental results on transition from lift-off (0.4 mm nozzle) to blow-off (0.3 mm nozzle) at storage pressure of about 10 MPa.

KEYWORDS: Blow-off, CFD, experiment, hydrogen jet, lift-off, simulation.

INTRODUCTION

There are three characteristics of flame stability i.e. lift-off velocity, lift-off height, and blow-out velocity. If the release rate is sufficiently low, a turbulent jet diffusion flame will stabilise at the nozzle exit. With the increase of the flow velocity at the point when the critical exit velocity will be exceeded, the jet flame will detach from the orifice and re-stabilize at some axial distance downstream the nozzle. This is known as the flame lift-off phenomenon and the critical exit velocity at which it occurs is called the lift-off velocity. Lift-off height is the distance between the nozzle exit and flame base. A number of studies, such as [1]–[5], have investigated the stable lifted flame reaction zone structures that settle at moderate downstream positions. If the release velocity continues to increase, the reaction zone starts to move further downstream and eventually it reaches the region that could no longer support combustion due to the low fuel concentration. This condition is known as the flame blow-out or blow-off and it leads to flame extinction. The blow-off condition has been investigated by [6]–[10]. The base of the lifted flame is assumed to be stabilized by propagation of a turbulent premixed flame against the flow where the flame propagation velocity equals to the opposite flow velocity.

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Research performed by [11]–[14] addressed the related elements of flame blowout; further overview of the research on blowout is contained in [10]. Recently, in [15] it was reported on lifted flames near blowout, with detailed comments on a triple flame in the pulsating region, and described a proposed mechanism of flame pulsation and blowout. The relation between flame blow-off and release pressure and orifice diameter has been investigated experimentally in [16] and [17]. The combustion states of the flame were investigated with various nozzle diameters and the release pressures of hydrogen. Nevertheless, the mechanisms that cause a jet-flame blow-out are still not completely understood and remain the area of active research.

The need of this study is to understand the phenomena more deeply and aid in safety considerations for the design of TPRD. The model that has been used here was successfully applied recently [18] to simulate the hydrogen spontaneous ignition during sudden release into air and in the numerical study of indoor jet fire regimes [19]. The notional nozzle theory for under-expanded jets [20] is applied as a part of the CFD modelling approach.

EXPERIMENTAL SETUP AND RESULTS

A series of three experiments were performed at *Toyota Technological Institute* to study lift-off and blow-off phenomena of under-expanded hydrogen jet fire. Figure 1 shows the experimental setup, where hydrogen gas flows from a storage vessel to the release nozzle through a stainless steel pipe with internal diameter of 4.0 mm and exits the nozzle when electric needle valve operates.
The ignition of the hydrogen jet was initiated by a pilot burner, which was installed at 0.2 m from the nozzle exit. The maximum storage pressure was 14.7 MPa. The pressure gauge installed just before the nozzle exit recorded the release pressure in each experiment. In experiments there were three nozzle diameters used: 0.3 mm, 0.4 mm and 0.5 mm. These nozzles were connected to a stainless steel pipe with 4 mm Swagelok tube fittings. The Schlieren method with high speed camera was used for observation of the flame behaviour. Schlieren method is based on visualization of density gradients, making possible to see areas with density change caused by shock waves, hydrogen jet in air and combustion.

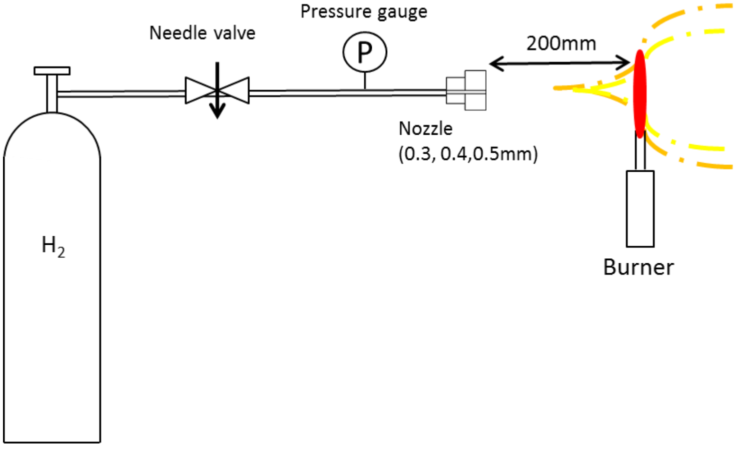

Figure 1. Experimental setup outline.

The detailed outline for flame visualisation installation is presented in Fig. 2. This is an optical system that utilised neodymium-doped yttrium orthovanadate (YVO_4) solid state laser with wave length of 532 nm, a slit, two concave mirrors (*d*=150 mm), a knife edge and a high speed camera.

The cross in yellow circle in Fig. 2 represents the jet as if one looks at it from the direction side of the jet towards nozzle exit. The laser passing through the slit then reflects from the concave mirror 1 generating the beam that goes through the nozzle and capturing the near nozzle area where lift-off expected. Then, the image of the beam that went through the area of interest reflects from the concave mirror 2 and goes to the high speed camera with frame rate of 2000 frames per second. The total duration of each experiment from the moment of opening the valve to the moment of its closure was set to 2 seconds. The results of these experiments are as follows: nozzles with diameter 0.4 and 0.5 were able to sustain the flame, the nozzle with 0.3 diameter ignition did not even appear on video filmed by camera.

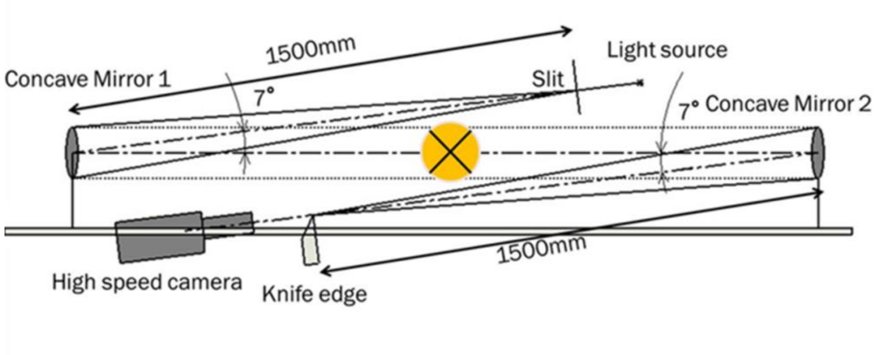

Figure 2. Schematic of experimental Schlieren system.

CFD MODEL GEOMETRY AND GRID

The renormalization group (RNG) k-ε turbulence model is applied similar to what is been used for simulation of hydrogen jet fires indoors, and fully described in [19]. In order to reproduce the lift-off and blow-off phenomena the solver with incompressible-ideal-gas for calculation of density was applied same as was used in previous study [19].

The eddy dissipation concept (EDC) model for simulation of combustion was applied, which is an extension of the eddy dissipation model that includes a chemical reaction mechanism in a turbulent flow [21]. The detailed chemical reaction mechanism [22] of hydrogen combustion in air employing 37 elementary reactions and 13 species is applied. This is the same implementation of the model as that in numerical simulations of spontaneous ignition of hydrogen during sudden release into T-shaped pressure relief device published recently [18]. The simulations [18] reproduced experimental data on the pressure limit for spontaneous ignition that proves the predictive power of the model and the simulation approach applied.

Simulation was performed using ANSYS Fluent pressure-based solver with SIMPLE pressure-velocity coupling algorithm which is recommended for a steady-state flow calculations. The spatial discretization for the gradient was Green-Gauss cell based, the second order for pressure, second order upwind for momentum, species and energy, and first order upwind for k and ε. The transient formulation was the first-order implicit and the gravity forces were applied. In order to improve the general solution behaviour the high order term relaxation (HOTR) of all vaiables at factor of 0.75 was used.

The computational hexahedral grid with 257,327 control volumes presented in Fig. 3 has a parallelepiped shape with dimensions of $HxWxL$=11x11x30 cm. The symmetries bisected the domain into quarters in order to save the computational time and have a better resolution of the grid in the vicinity of the nozzle. However, Fig. 3 shows the full grid with mirrored symmetries.

The nozzle exit location was 10 from the boundary towards the release direction. During grid generation all recommendations, best practices and requirements were applied as stated in [23]. The square nozzle was of the same area as circle and was resolved by 5 cells. In all simulations the real nozzle was replaced by the notional nozzle to simulate under-expanded release as described in [20]. The parameters on the notional nozzle were calculated using online engineering tool "Cyber-laboratory" available from [24]. Conditions at the nozzle exit together with parameters of the turbulence and the notional nozzle are presented in Table 1. The use of turbulent intensity of 25% and turbulence length scale equivalent to 7% of the notional nozzle diameter provided the closest agreement with experimental observations in [25], same conditions applied in this study based on previous experience. The same grid was used in all simulations; the notional nozzle diameter has been changed by the grid scaling for each case.

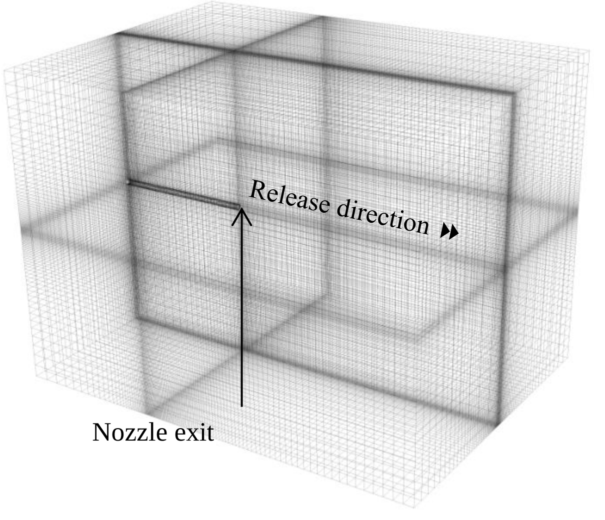

Figure 3. Computational grid, 3D view.

Table 1. Conditions at the nozzle exit.

Nozzle Ø, mm	Exit pressure, MPa	Release velocity, m/s	Notional nozzle Ø, mm	Temperature at the nozzle, K	Length scale, 7%	Turbulent intensity, %
0.3	10.8		2.2		0.137	
0.4	11.2	1188.3	2.99	243	0.185	25
0.5	11.4		3.77		0.234	

RESULTS AND DISCUSSION

All CFD calculations were performed in the same manner and included several steps. The first was the calculation of hydrogen steady state unignited jet. The second was the ignition phase in which the temperature of 3000 K was patched. As soon as OH radical concentration in the composition of air reached above 1% by volume, the ignitor was deactivated. When the ignitor was switched off, the flame behaviour was observed in transient mode until flame was stabilised or blown-off.

Figure 4 shows the velocity (left) and hydrogen mole fraction (right) distribution along the release centreline in steady state unignited solution just before ignition step. It can be seen that with reduction of release diameter velocity increases and concentration decreases along the jet centreline. Further from the jet centreline to the sides the concentration decreasing which can explain the fact that in the case of 0.3 mm nozzle the hydrogen-air mixture concentration was not sufficient at the places where the flame velocity could overcome velocity of the flow which resulted in blow–off the case with 0.3 mm.

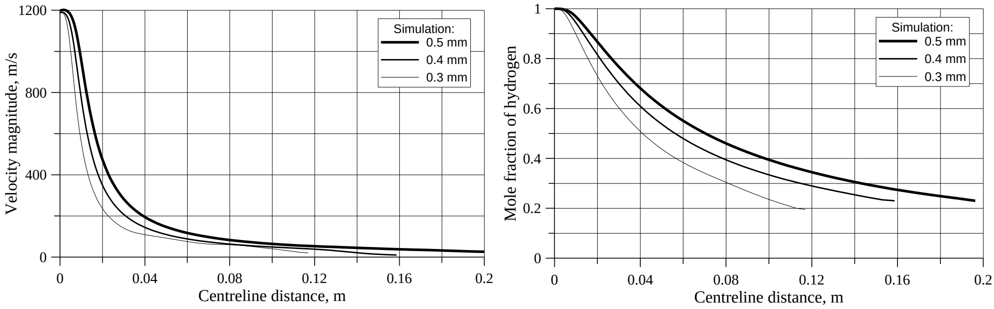

Figure 4. Simulated centreline distribution of velocity (left) and mole fraction of hydrogen (right).

Figure 5 shows the comparison of experimental Schlieren snapshot with a 2D cross-sections of simulated density contours along the jet centreline. This is the only available experimental information about phenomena, such important parameter as jet velocity has not been measured during experiment, and therefore, only visual comparison is presented here. The steady state solution obtained by transient simulation for nozzle diameters 0.4 mm is shown in Fig. 5 (left) and the one for nozzle diameter of 0.5 mm is shown in Fig.5 (right). Simulations demonstrate a good agreement with experiments. The two upper rows of snapshots (Fig. 5) show the comparison of experiments with simulations. The shown values of lift-off distances in experiments are indicative and fluctuate within about 10-15% in the experiments. The simulation values do not show fluctuations and the lift-off distance is fixed within the error of visual estimate. The bottom row of snapshots in Fig. 5 shows that the experimental and simulated snapshots overlap perfectly. The CFD model was able to reproduce not only the shape flame and the lift-off distance. The most important is that the simulations reproduced experimentally observed phenomenon of flame blow-off at transition from 0.4 mm diameter nozzle to 0.3 mm nozzle. In simulation, after ignition, the flame propagates from the ignition point towards the nozzle and then stabilises at lift-off distance for 0.4 and 0.5 mm nozzle, similar to the experiments.

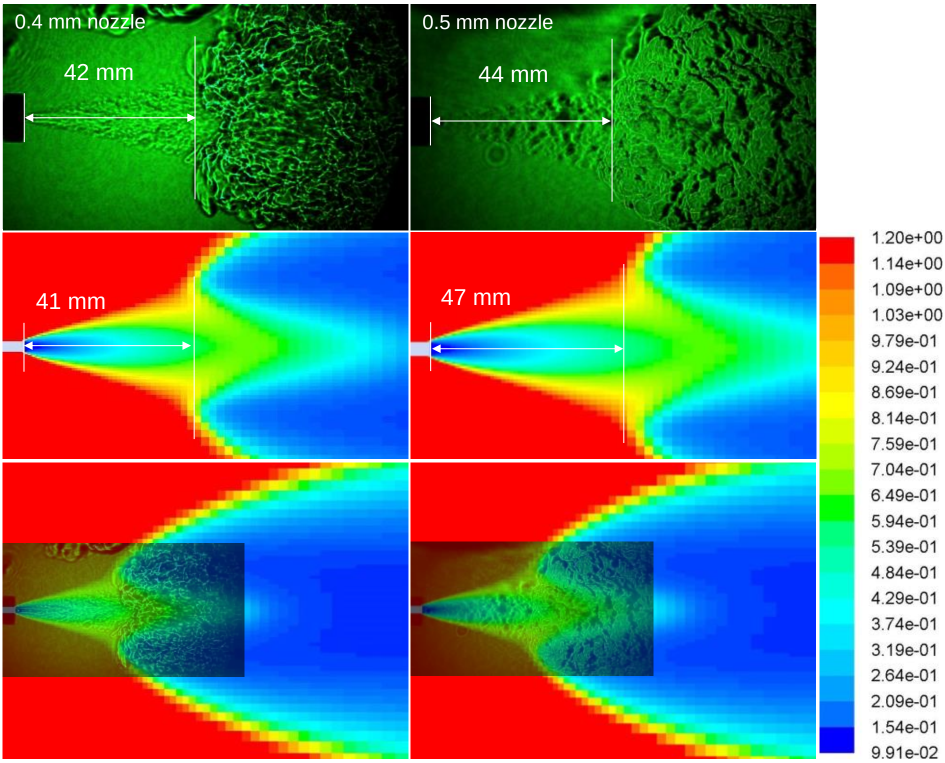

Figure 5. Experimental Schlieren snapshot versus simulated density cross-section snapshot along jet centreline for 0.4 mm diameter nozzle (left) and 0.5 mm nozzle (right).

The model capability to predict blow-off is shown in Fig. 6. The simulated results of hydrogen and OH mole fractions and temperature are shown at the same time of 1 s after ignition. It can be seen that the distance from the domain boundary is different for each experiment. This is due to domain scaling. For both cases, 0.4 and 0.5 mm, the steady-state flame lifted from the nozzle at the lift-off distance. However, for the case with 0.3 mm orifice, parameters of OH, temperature and H2 show that there is no combustion and slight traces of OH shows that when the ignition was switched off, the flame has been blown away.

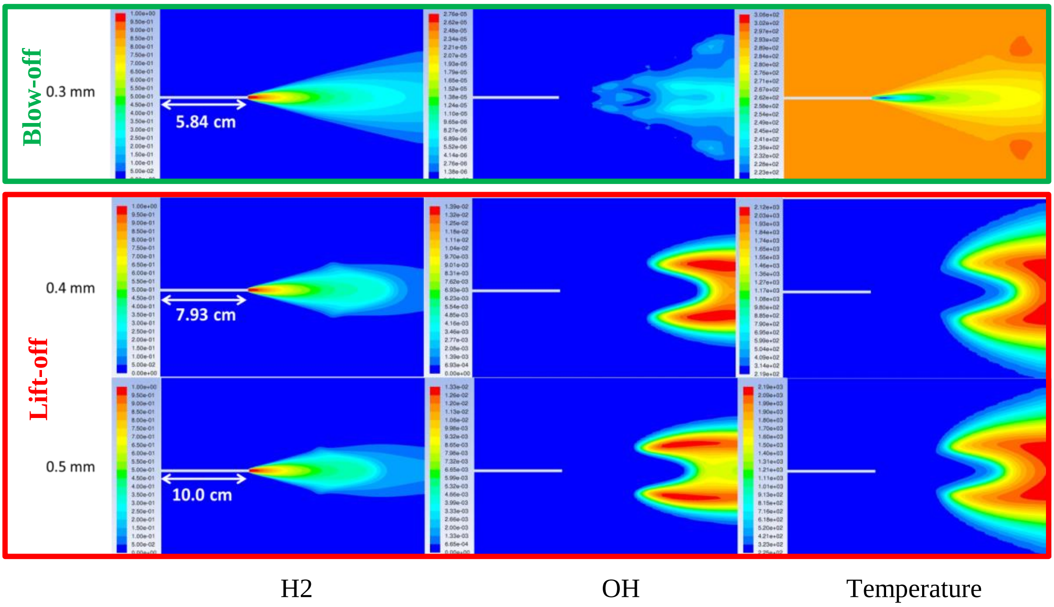

Figure 6. Simulated cross-section snapshots of mole fractions of hydrogen, hydroxyl and temperature across the centreline of the pipe for experiments with 0.3, 0.4 and 0.5 mm.

CONCLUSIONS

Numerical experiments were performed to simulate the lift-off height and blow-off of hydrogen non-premixed turbulent flame for nozzle diameters of 0.3 mm, 0.4 mm and 0.5 mm. The simulations closely reproduced the experimentally observed lift-off height for 0.4 mm and 0.5 mm diameter nozzles, and the blow-off phenomenon for 0.3 mm nozzle diameter. It can be concluded, that the used CFD model with incorporated notional nozzle theory is an efficient tool for hydrogen safety engineering, able to reproduce the lift-off and blow-off phenomena for under-expanded jets in a comparatively short CPU time.

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