VALIDATION OF A HYDROGEN JET FIRE MODEL IN FDS

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ABSTRACT

Hydrogen jet fire occurs with high probability when hydrogen leaks from high-pressure equipment. The hydrogen jet fire is characterized by its high velocity and energy. Computational Fluid Dynamics (CFD) numerical analysis is a prominent way to predict the potential hazards associated with hydrogen jet fire. Validation of the CFD model is essential to ensure and quantify the accuracy of numerical results. This study focuses on the validation of the hydrogen jet fire model using Fire Dynamic Simulation (FDS). Hydrogen release is modeled using high-speed Lagrangian particles, released from a virtual nozzle, thus avoiding the modeling of the actual nozzle. The mesh size sensitivity analysis of the model is carried out in a container-size domain with 0.04m – 0.08m resolution of the jet. The model is validated by comparing gas temperatures and heat fluxes with test data. The promising results demonstrated that the model could predict the hazardous influence of the jet fire.

1.0 INTRODUCTION

1.1 Background

Hydrogen is regarded as a future optional fuel for vehicles due to its high specific energy and zero carbon emissions. Hydrogen vehicles usually carry a hydrogen tank at a pressure of up to 70 MPa. In order to improve the safety of hydrogen vehicles, a thermal pressure relief device (TPRD) is applied to a vehicle to clear up tanks. The TPRD device is activated when the surrounding temperature rises to about 110 ºC, causing hydrogen to be released from a tank with a small-size orifice. Furthermore, immediate ignition by, e.g., an external fire, leads to a hydrogen jet fire.

Hydrogen jet fire is distinctly different from hydrocarbon fire, e.g., petroleum and methane fire. For example, the heat of combustion of hydrogen is significantly higher than liquid petroleum gas (LPG), causing the high temperature of the jet fire flame [1]. Due to their non-sooting nature, hydrogen flames emit less heat radiation than hydrocarbon flames, and heat transfer mainly occurs as convection. This fact also implies that a hydrogen jet fire is rather invisible to humans because it is mainly emitting hot water vapor producing heat radiation in the infrared. Therefore, hydrogen jet fire as a vital fire phenomenon is of great interest to explore.

Up to now, some tests have been performed to investigate the properties of hydrogen jet fire [2-4]; however, most of them are limited owing to difficulties in real hydrogen jet fire tests, such as exorbitant costs and security contemplations. Thus, to fill gaps, alternative techniques like computational fluid dynamic (CFD) simulation are considered. Several CFD software are available for simulating jet fires, including FLUENT, FLACS, and FDS. Muthusamy et al. [5] used FLACS to simulate nine impinging jet fire scenarios with different orifice diameters and geometrical configurations. According to the results, the heat flux from a smaller orifice release is more consistent with the test value, while a larger orifice release may result in higher heat flux. This is because a larger orifice release could improve the convection heat flux by a more transient release. Li. et al. [6] built a hydrogen car model in Fluent to study the safety separation distance for a 4.2 mm TPRD release downwards. Their simulation results showed that the minimum distance for 35 MPa and 70 MPa tanks is 10m and 12m, respectively. Rengel et al. [7] explore the characteristics of sonic jet fires in FLACS-Fire, FDS, and FireFOAM. Comparing the fire temperature and heat flux in different software, FLACS-Fire estimated the fire temperatures more accurately, while both FDS and FireFOAM under-estimated the fire temperatures. On the other hand, the heat flux was reasonably predicted in FDS and FLACS-Fire, but overestimate in FireFOAM. Wang et al. [8] studied the radiation characteristics of under-expanded hydrogen jet fires using FireFOAM by applying a large eddy dissipation method.

In view of the previous works, CFD simulation is shown to be an efficient approach to analyzing hydrogen jet fire behaviors, especially for large-size fire scenarios (vehicle fires, tunnel fires, building fires, and so on). Furthermore, to get reliable and accurate performances of, validation of the CFD model is crucial before simulating any fire scenarios. FDS is one of the essential programs for studying fire behaviors owing to well documented and relatively short simulation time. However, the algorithms in FDS have some limitations, like low Mach number due to the incompressible fluid assumption. Therefore, a new simplified model to overcome these limitations is of great interest to build in FDS.

1.2 Aim

In light of the pressure and velocity of the hydrogen jet fire, it is divided into three regimes: traditional buoyancy-controlled, traditional momentum-dominated ‘plateau’ for expanded jets, and momentum-controlled under-expanded jet fire [9]. Considering the safety issues in a vehicle caused by the high pressure and velocity of a jet fire, the momentum-controlled under-expanded hydrogen jet fire will be investigated in this study by using FDS. This hydrogen jet fire occurs when hydrogen leaks from a tank in a vehicle and is ignited immediately. Moreover, the impingement of hydrogen jet flames on the floor happens when the direction of a TPRD device in a vehicle is directed downwards, further exacerbating the safety issues associated with hydrogen leakage in a vehicle.

Taking into consideration the limitations of the FDS software and the insurmountable computational cost of resolving simultaneously the different length scales of the nozzle/leak and the affected environment, a simplified FDS model is proposed in this study. It is using Lagrangian particles to introduce the hydrogen into the computational domain. In the model, the real nozzle of a hydrogen tank is not simulated explicitly. This simplifies the computational problem significantly as we do not need to resolve the very small-diameter and high-speed exit flow of the nozzle. Instead, fuel inflow is treated as a sub-grid scale phenomenon. The model is validated by comparing the simulation results with test data [10, 11]. Finally, through these validation processes, some guidance regarding modeling a hydrogen jet fire in FDS is proposed.

2.0 HYDROGEN JET FIRE MODEL

2.1 Brief introduction of the test

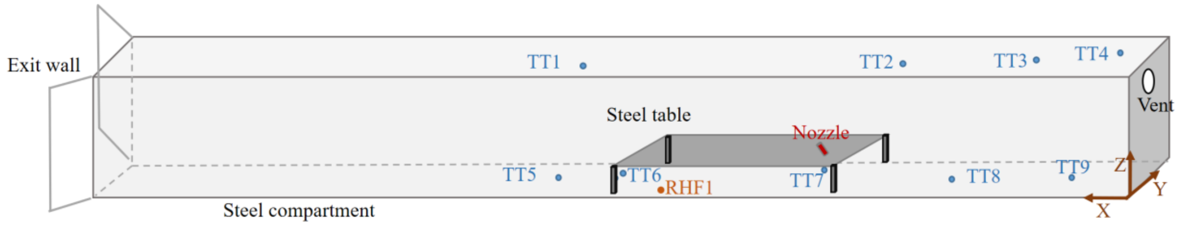


Figure 1 Experimental setup showing the measurement points after [11]. TT are thermocouples and RHF is a heat flux sensor. (see also Table 1)

In this study, models of hydrogen jet fire are developed in FDS according to the literature [10, 11], and the test setup can be seen in Figure 1. ‘TT’ refers to the thermocouple, and ‘RHF’ refers to the radiative heat flux sensor. The position of nine thermocouples and one radiative heat flux sensor are listed in Table 1.

Table 1 Temperature and heat flux sensors location [10, 11] (see also Figure 1)

Sensor	X (m)	Y (m)	Z (m)	Sensor	X (m)	Y (m)	Z (m)
TT1	6.25	1.12	2.105	TT6	6.33	0.868	0.198
TT2	2.32	1.12	2.105	TT7	4.6	0.86	0.2
TT3	1.06	1.12	2.105	TT8	3.31	0.074	0.235
TT4	0.11	1.12	2.105	TT9	1.03	0.08	0.235
TT5	7.2	0.08	0.235	RHF1	6.08	0.04	0.235

The University of South-Eastern Norway kindly provided the experimental test results for this validation study [10, 11]. The experimental tests are carried out in a steel compartment with a dimension of 11.885 m × 2.24 m × 2.285 m (length × width × height). The insulation material thickness covering the walls and ceiling is 0.07 m. The steel table shown in Figure 1 is used to imitate a hydrogen car with a dimension of 1.965 m × 0.73 m × 0.25 m (lenght × width × height). The hydrogen nozzle is mounted under the steel table, 0.18 m above the floor.

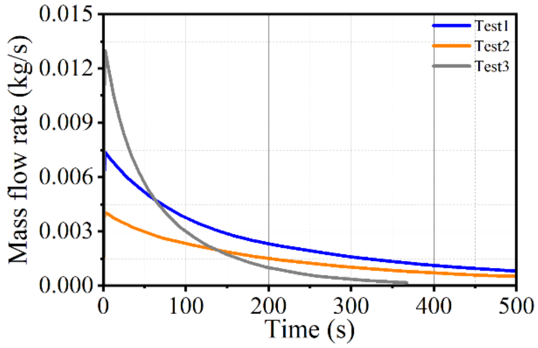


Figure 2 Mass flow rate of the nozzle after [10, 11]. Test 1: 0.5mm nozzle/698 bar; test 2:0.5mm nozzle/360 bar; test 3: 1mm nozzle/ 357 bar.

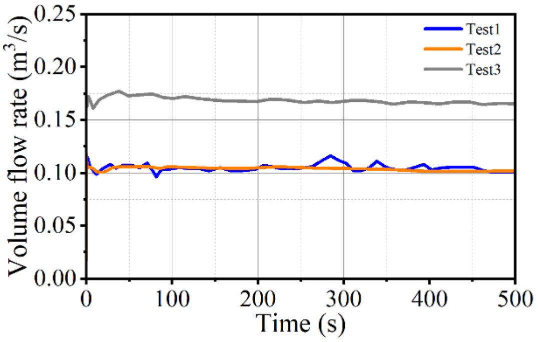


Figure 3 Volumetric flow rate of the ventilation after [10, 11]. Test conditions as in Figure 2.

In the test, one steel wall opens (the exit wall), and the ventilation pipe is on the opposite wall of the exit wall, located 0.05 m from the ceiling with a 0.315 m outlet diameter. The function of this ventilation pipe is to suck out the air and the hot combustion products. The temperatures at nine positions are measured (see Figure 1 and Table 1). The mass flow rates of the nozzle and the volumetric flow rates of the vent are shown in Figure 2 and Figure 3, respectively.

Three different hydrogen jet fire experiments are discussed in this study. Hydrogen is released with 45° nozzles in three tests. The difference among these tests is the nozzle diameter, initial tank pressure, and jet duration. The hydrogen jet duration in test 1 and test 2 is 500 s with a 0.5 mm nozzle diameter. The initial tank pressure in test 1 and test 2 are 698 bar and 360 bar, respectively. Test 3 involved a hydrogen jet duration of 367 s with an initial tank pressure of 357 bar and 1 mm nozzle diameter.

2.2 CFD model of hydrogen jet fire

FDS is developed by the National Institute of Standards and Technology (NIST) with the aim of solving practical fire issues and researching fundamental fire dynamics and combustion [12]. Version 6.7.9 of FDS, a widely-used and freely available program for simulating fire and smoke propagation [13], was utilized in this study. Large Eddy Simulation (LES), a typical mathematical method in FDS to solve turbulence, was employed in the model to investigate the hydrogen jet fire in this study. The LES method enabled obtained results in FDS by solving every conservation equation with numerical methods [14]. The primary conservation equations of LES include mass conservation, energy conservation, and momentum conservation [15]. Since the code was initially designed to handle low-speed flow cases, momentum-controlled flows cannot be directly simulated in FDS. Therefore, a simplification of the under-expanded jet fire has been necessary for the FDS simulation.

The numerical domain is 12 m long, 2.24 m wide, and 2.28 m high. At solid boundaries, one-dimensional heat conduction was used to calculate the heat transfer to the steel walls, the fire plate and the insulation material, having thermal conductivities of 45.8 W/mK, 0.05 W/mK and 0.05 W/mK, respectively. The hydrogen release was simulated as a spray of liquid hydrogen particles with an initial speed of 200 m/s, a median droplet diameter of 1000 μm, an initial temperature of -260 ^{o}C and a spray angle of 5^{o}. The number of droplets inserted every second at the active nozzle was 10000. The initial mass flow rate was 0.004kg/s and the initial volume flow rate was 0.11 m^{3}/s for the case study model in this section. The combustion of the evaporated hydrogen gas was simulated using a mixing-controlled, Eddy Dissipation Concept model for the chemical source term. Furthermore, to prevent the hydrogen from igniting as soon as it exits the nozzle, an artificial auto-ignition temperature of 250 °C was used to prevent combustion at low-temperature regions. Due to the resolution constraints, this temperature is lower than the actual hydrogen auto ignition temperature. The nozzle of the FDS model can be seen in Figure 4.

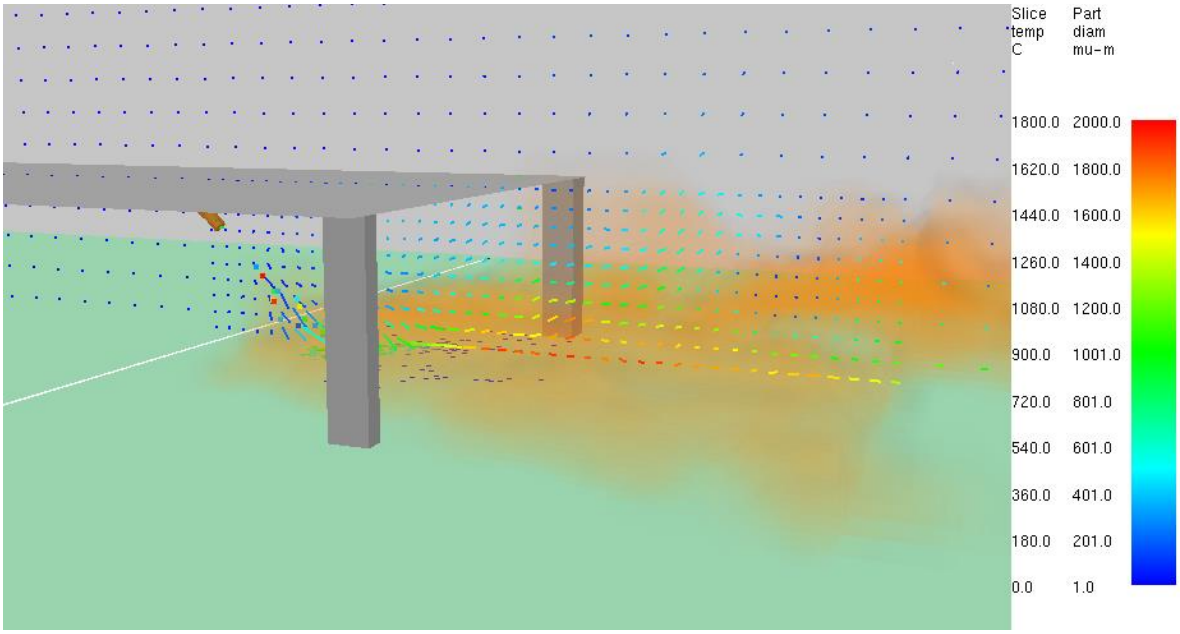


Figure 4. FDS model of the hydrogen jet flame, with instantaneous velocity vectors, gas temperature in ^{o}C, and particle sizes in µm.

2.3 Mesh study

A good balance between accuracy and computational costs is required to run the FDS simulation in a reasonable time. The area near the nozzle, where a higher momentum is expected, is discretized with a smaller mesh than the remaining domain. A mesh sensitivity study with 5 different mesh sizes is carried out, as shown in Table 2. Mesh screenshots around the nozzle are shown in the third column. The smallest mesh size is 0.04 m, and the maximum mesh size is 0.08 m. Figure 5 exhibits the total energy of this nozzle model at different mesh sizes from the experimental test 2. The formula of total heat energy [16] is shown in Equation (1). The calculated total energies found with grids 1, 2, and 3 are all close to the test 2 value, which is around 91 MJ. When the number of grid cells decreases, the total energy value is gradually moving away from the dashed dot line. Thus, taking into account the accuracy and computational cost in the FDS simulation, grid 2 can be used for later calculations. Figure 6 is the temperature slice of test 2 under grid 2 at different times. In Figure 6, the slice is located at the width center of the steel compartment. The maximum temperature is above 1500^{o}C, and the temperature decreases as the jet duration increases.

$$Q = \int \dot{m} \Delta H \, dt \,, \qquad (1)$$

Where Q – the total energy, J; $\dot{m}$ – the burning rate of hydrogen, kg/s; ΔH – the hydrogen heat of combustion, J/kg.

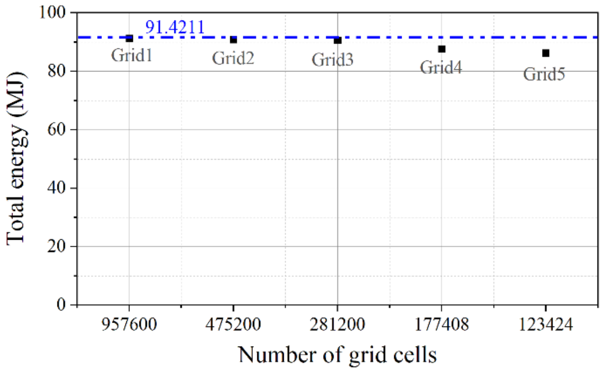
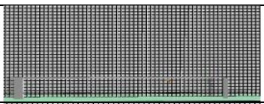
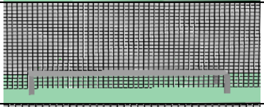
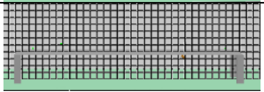
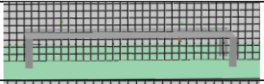
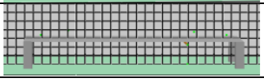


Figure 5 Heat energy under different cell sizes

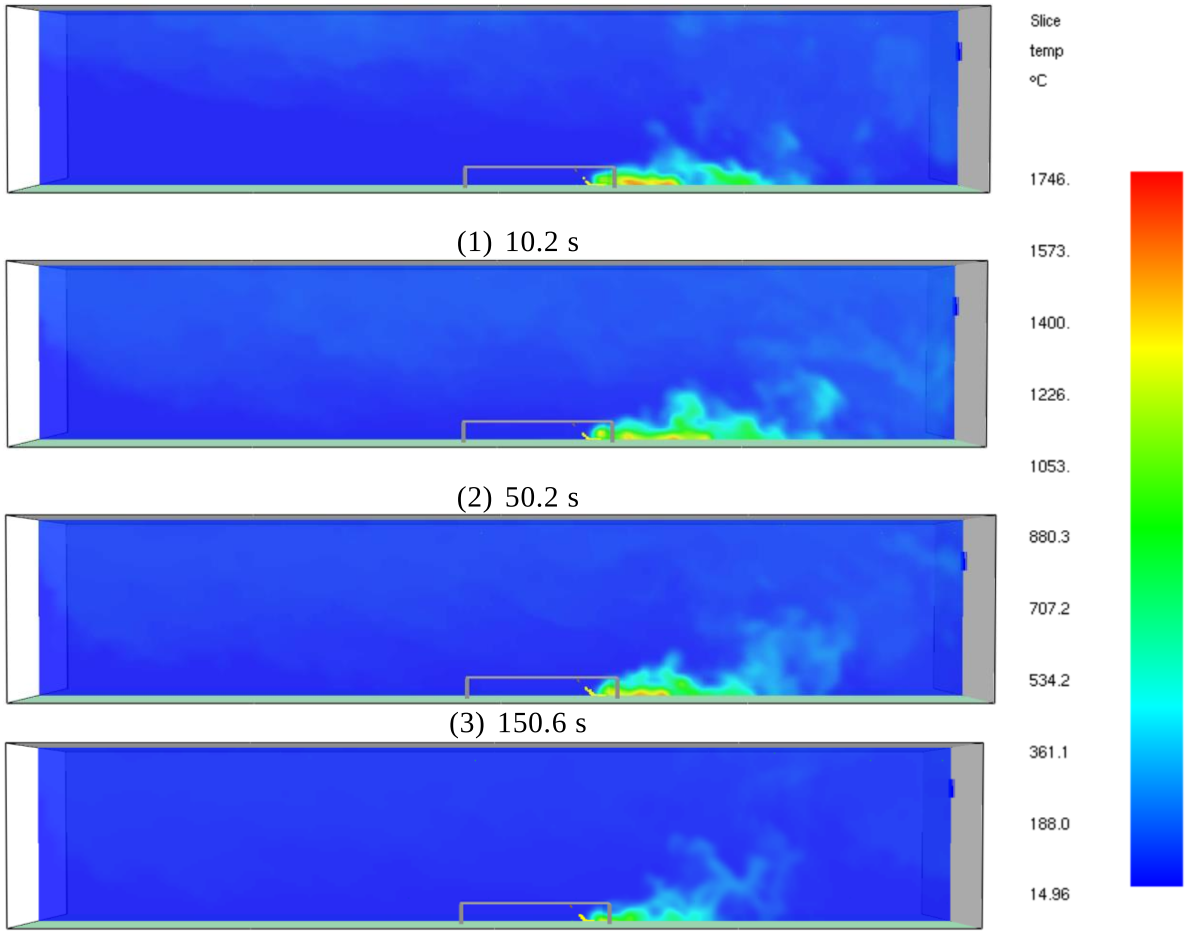
Table 2. Information of different grids

Cases	Grid size closed the nozzle X(m) x Y(m) x Z(m)	Grid diagram	Total number of grid cells in the nozzle model
Grid1	0.04x0.04x0.04		957600
Grid2	0.05x0.05x0.05		475200
Grid3	0.06x0.06x0.06		281200
Grid4	0.07x0.07x0.07		177408
Grid5	0.08x0.08x0.08		123424

3.0 MODEL VALIDATION

Temperatures of nine thermocouples and one heat flux measurement are compared with the experimental test results, as shown in Figure 7. The differences between the three tests and models are the mass flow rate of the nozzle and the volume flow rate of the ventilation. All of these simulations in this section adopt grid 2 as the mesh size.

Figure 7 (1)-(4) shows the thermocouple temperature close to the ceiling of the steel compartment. The comparisons demonstrate good agreement between the FDS simulation and test results. The maximum temperature is in TT3, approximately 324.2°C in test 3, and 343.9°C in FDS3. The temperature of thermocouples located behind the nozzle and close to the ground are displayed in Figure 7 (5)-(6). The temperature curves of TT5 and TT6 are very similar to the test results. The maximum temperature of TT5 and TT6 is less than 70°C. Simulation results of thermocouple TT8 are displayed in Figure 7 (8). The results indicate that only the simulation result of Test 1 (FDS1) is close to the test data. For the thermocouple TT9, located in front of the nozzle and near the ventilation, simulations of test 1 could predict the trend of gas temperature, and all of the FDS models could estimate the maximum gas temperature. In addition, maximum heat flux behind the nozzle could be predicted in FDS2 since the peak value are almost very close to the test data, while FDS1 overestimates the maximum heat flux (see Figure 7 (9)).



(1) 10.2 s

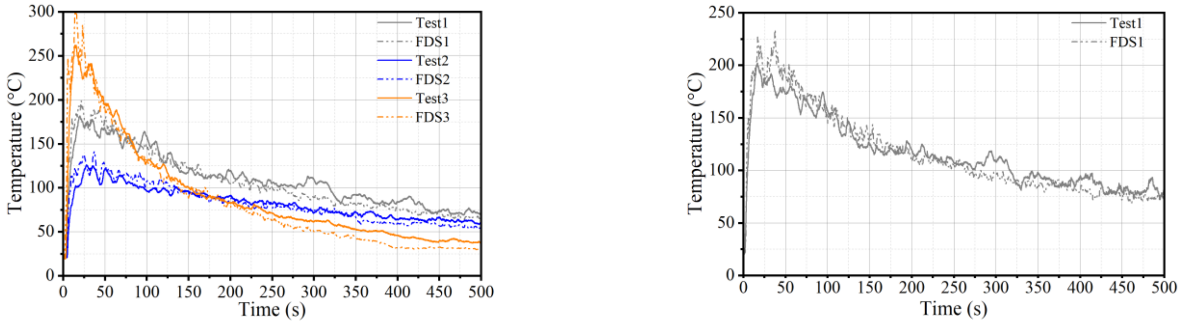
(2) 50.2 s

(3) 150.6 s

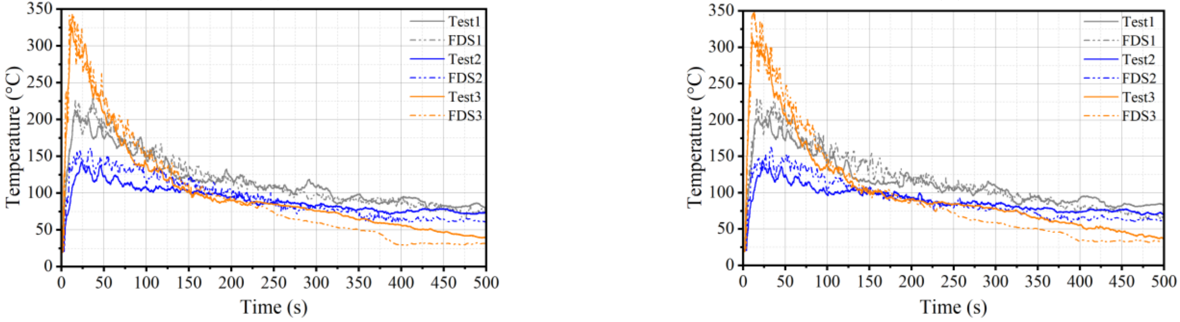
(4) 400.1 s

Figure 6 Temperature slice of grid 2 at different times.

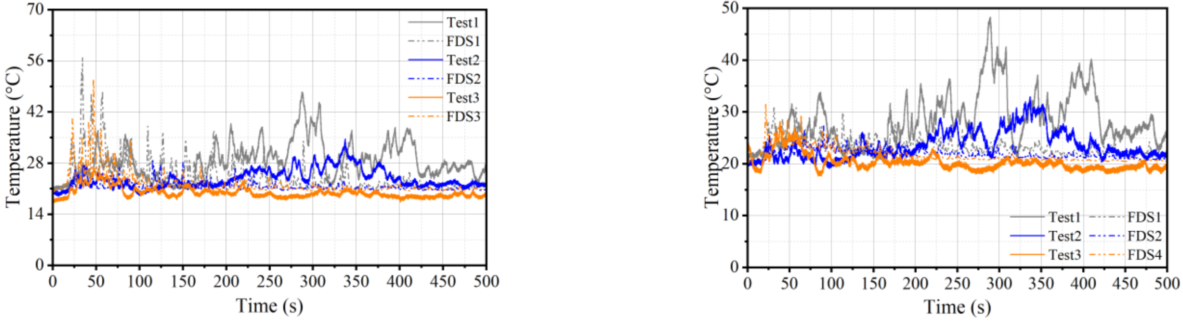
In Figure 7, TT7 of FDS simulation is always highly overestimated at the beginning of the simulation. But after 75 s, the temperature curve of FDS1 is similar to the test curve. This dissimilarity may be caused by the lower Mach number limitation in FDS. In the actual test, the flow close to the nozzle is larger than the sound speed, which exceeds the Mach number limitation of FDS. Furthermore, fine details of the nozzle and thermocouple placement and other geometrical factors may have been modeled with less-than-necessary accuracy, causing the simulation results to be lower or higher than the actual test value.



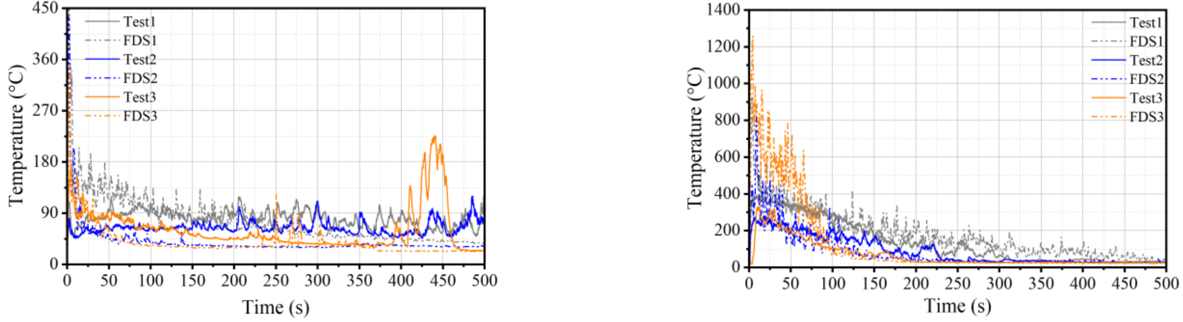
(1) TT1 (2) TT2



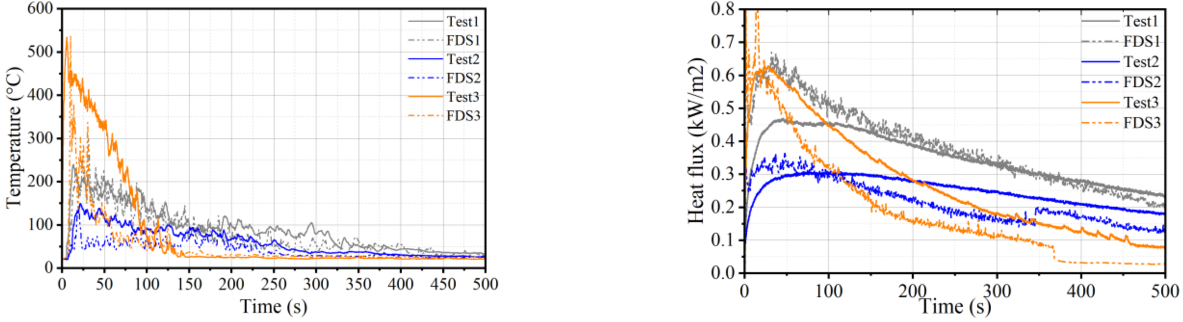
(3) TT3 (4) TT4



(5) TT5 (6) TT6



(7) TT7 (8) TT8



(9) TT9 (10) RHF1

Figure 7 Comparison of the experimental tests [10, 11] and the FDS simulation results

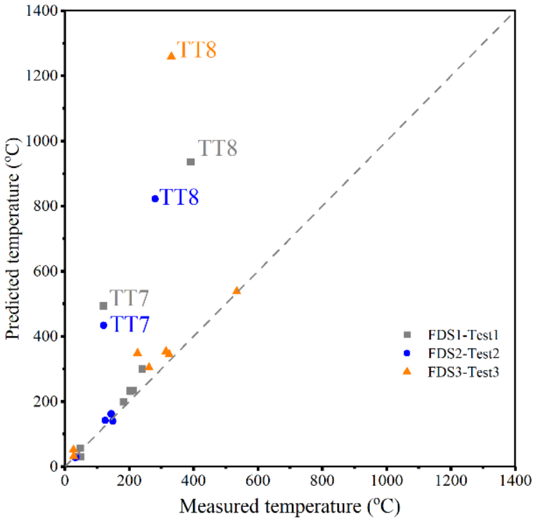


Figure 8 A comparison of predicted and measured maximum temperature for the different fire scenarios in the tests 1, 2 and 3.

Figure 8 compares measured and predicted maximum temperatures for three fire scenarios. Most of the FDS thermocouple models predict well the maximum temperatures among different fire scenarios. Only a few FDS thermocouples highly overestimated the maximum temperature, e.g., TT8 thermocouple in all of simulations, TT7 in FDS1 and FDS2, the estimated maximum temperature in FDS3 is approximately three times the experimental temperature.

4.0 CONCLUSION

A simplified virtual nozzle FDS model is proposed to simulate hydrogen jet fires. The high-speed hydrogen jet is modelled applying Lagrangian particles that carry necessary mass and momentum. The particles evaporate quickly producing a gas phase jet. Numerical results concerning the gas temperature and heat flux are compared with experimental test data for the hydrogen jet fire. The results from this analysis are summarized below:

(1) The gas temperature close to the ceiling is more accurate than the gas temperature close to the nozzle in the FDS model. This may be due to the fact that the FDS has limitations in simulating under-expanded flow with a high Mach number. Also, fine details of the nozzle and thermocouple placement and other geometrical factors may have been modelled with less-than necessary accuracy.
(2) The gas temperatures near the ceiling and behind the nozzle are consistent with the test data, indicating that the modelling approach provides an accurate and efficient method for engineering CFD of hydrogen jet fire consequence analysis.
(3) In this simulation, the trend of heat flux behind the nozzle is in good agreement with the test data, and the model can therefore be used to estimate the heat flux of hydrogen jet fire.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the financial support provided by the Fuel Cells and Hydrogen 2 Joint Undertaking (now Clean Hydrogen Partnership) under Grant Agreement No 826193. The authors gratefully acknowledge the support from the European Union's Horizon 2020 Research and Innovation program, Hydrogen Europe and Hydrogen Europe Research, as well as the Finnish Fire Protection Fund (Palosuojelurahasto). The authors gratefully acknowledge the experimental test data provided by the University of South-Eastern Norway.

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