

# THERMAL RADIATION FROM CRYOGENIC HYDROGEN JET FIRES

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## ABSTRACT

The thermal hazards from ignited under-expanded cryogenic releases are not yet fully understood and reliable predictive tools are missing. This study aims at validation of a CFD model to simulate flame length and radiative heat flux for cryogenic hydrogen jet fires. The simulation results are compared against the experimental data by Sandia National Laboratories on cryogenic hydrogen fires from storage with pressure up to 5 bar abs and temperature in the range 48-82 K. The release source is modelled using the Ulster's notional nozzle theory. The problem is considered as steady-state. Three turbulence models were applied, and their performance was compared. The realizable k- $\epsilon$  model showed the best agreement with experimental flame length and radiative heat flux. Therefore, it has been employed in the CFD model along with Eddy Dissipation Concept for combustion and Discrete Ordinates (DO) model for radiation. A parametric study has been conducted to assess the effect of selected numerical and physical parameters on the simulations capability to reproduce experimental data. DO model discretization is shown to strongly affect simulations, indicating 10x10 as minimum number of angular divisions to provide a convergence. The simulations have shown sensitivity to experimental parameters such as humidity and exhaust system volumetric flow rate, highlighting the importance of accurate and extended publication of experimental data to conduct precise numerical studies. The simulations correctly reproduced the radiative heat flux from cryogenic hydrogen jet fire at different locations.

Keywords: CFD, jet fire, cryogenic, hydrogen, radiative heat transfer

## 1 INTRODUCTION

Cryo-compression is a competitive technique when storage of large quantities of hydrogen is needed [1]. Understanding of consequences of potential accidents with cryogenic release of hydrogen is fundamental to protect life and prevent property loss. Predictive models are needed for hydrogen safety engineering to calculate hazard distances in case of cryogenic unignited and ignited releases. Only few experiments have been performed to investigate thermal hazards from cryogenic jet fires. Friedrich et al.'s experiments performed in Germany concerned releases with pressures from 7 to 35 bar abs and temperature in the range 34-65 K [2]. Flame stability, combustion regimes and thermal radiation were analysed. Health and Safety Laboratory (HSL) in UK performed experiments on 60 l/min spills of LH<sub>2</sub> combustion and estimated that the minimum safety distance to avoid damage from jet fire thermal effects shall be about 14 m [3]. The most recent experiments on cryogenic hydrogen jet fires were conducted at Sandia National Laboratories (SNL) in USA [4]. The radiative thermal heat flux and flame length were analysed for release temperature 37-295 K and pressures up to 6 bar abs. It was found that for a constant mass flow rate, the radiative heat flux increases for colder release temperatures, as consequence of the higher flame residence time. The present study simulated a selection of these experiments using Fluent as computational engine. Several numerical studies investigated liquefied (LH<sub>2</sub>) and cryogenic hydrogen unignited jets [5]–[7], while there is a lack of investigations on ignited releases, i.e. jet fires. Therefore, the aim of this study is to develop and validate a CFD model to predict radiative heat fluxes from a cryogenic jet fire at different locations from the flame. As part of the model development, a parametric study has been conducted, giving insights into the effect of several parameters and model assumptions on simulation results.

## 2 VALIDATION EXPERIMENTS

The experiments were conducted at the Turbulent Combustion Laboratory of SNL in USA. The main aim of the experiments was to investigate the ignition and flame characteristics of cryogenic under-expanded jet fires. The analysed scenarios were concerned with hydrogen releases with temperature in the range 37-295 K and pressure 2-6 bar abs. The release temperature and pressure were maintained constant during each test and monitored upstream the interchangeable orifice of diameter 0.75 mm or 1 mm or 1.25 mm. The hydrogen was released vertically upward in the laboratory equipped with an exhaust gases collection system. The facility geometry and dimensions are presented in Figure 1. The exhaust hood volumetric flow rate was varied from approximately 5100 to 7650 m<sup>3</sup>/h, depending on the hydrogen mass flow rate. The incident thermal radiation was monitored at 5 sensors located along the jet flame and at 0.2 m from the jet axis. The exact location of each sensor is shown in Figure 1. Additional experimental data to publication in [4] were provided by the authors through personal communication. The flame length was given as average of the visible and infrared (IR) cameras images. 5 tests out of the entire set of experiments performed by SNL have been selected for the CFD model development and validation. Table 1 shows the details of the experimental operating conditions of the selected tests. The orifice diameter for selected tests was 1.25 mm.

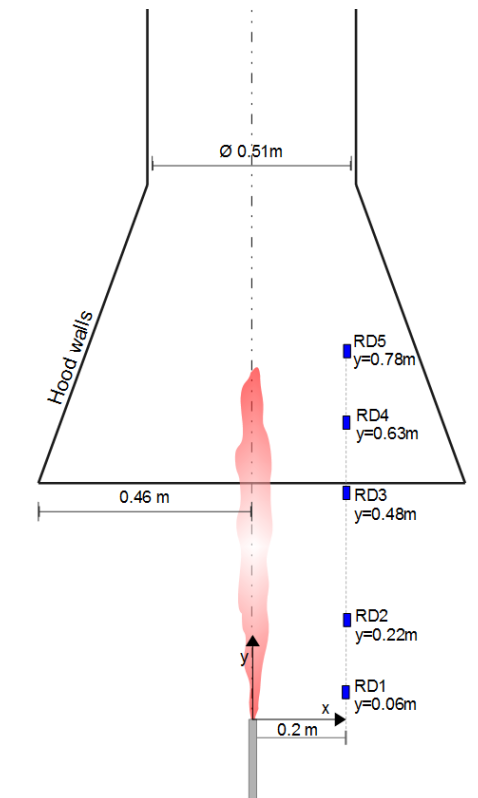


Figure 1. Scheme of the experimental set-up

Table 1. Experimental operating conditions of 5 validation tests [8]

| Test No. | Mass flow rate, g/s | Temperature, K | Pressure, bar abs |
|----------|---------------------|----------------|-------------------|
| 1        | 0.33                | 64             | 2                 |
| 2        | 0.38                | 48             | 2                 |
| 3        | 0.45                | 75             | 3                 |
| 4        | 0.56                | 78             | 4                 |
| 5        | 0.64                | 82             | 5                 |

### 3 MODEL AND NUMERICAL DETAILS

#### 3.1 Governing equations

The Reynolds-Averaged Navier-Stokes (RANS) conservation equations for mass, momentum, energy and species were solved:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0, \quad (1)$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i}(\mu + \mu_t) \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) + \rho g_i, \quad (2)$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial}{\partial x_i} (u_i (\rho E + p)) \quad (3)$$

$$= \frac{\partial}{\partial x_i} \left[ \left( k_t + \frac{\mu_t c_p}{Pr_t} \right) \frac{\partial T}{\partial x_i} - \sum_m h_m \left( - \left( \rho D_m + \frac{\mu_t}{Sc_t} \right) \frac{\partial Y_m}{\partial x_i} \right) + u_i (\mu + \mu_t) \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \right] + S_E,$$

$$\frac{\partial \rho Y_m}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i Y_m) = \frac{\partial}{\partial x_i} \left[ \left( \rho D_m + \frac{\mu_t}{Sc_t} \right) \frac{\partial Y_m}{\partial x_i} \right] + S_m. \quad (4)$$

where  $\rho$  is the density,  $t$  is the time,  $i, j$  and  $k$  correspond to the Cartesian coordinates and  $u$  to the velocity components,  $p$  is the pressure,  $\mu_t$  is the turbulent dynamic viscosity,  $\delta_{ij}$  is the Kronecker symbol,  $g_i$  is the gravity acceleration,  $E$  is the total energy,  $k_t$  is the thermal conductivity,  $c_p$  is the specific heat at constant pressure,  $Pr_t$  and  $Sc_t$  are the energy turbulent Prandtl and turbulent Schmidt numbers equal to 0.85 and 0.7 respectively,  $D_m$  is the molecular diffusivity of the species  $m$ ,  $Y_m$  is the corresponding mass fraction,  $S_E$  and  $S_m$  are the source terms in the energy equation and  $m$  chemical species transport equation.

Turbulence was accounted using the realizable  $k$ - $\varepsilon$  model [9], solving the transport equations for turbulence kinetic energy,  $k$ , and turbulent dissipation rate,  $\varepsilon$ , as follow:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \rho \varepsilon - Y_M, \quad (5)$$

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \frac{\partial(\rho \varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + \rho C_1 S \varepsilon - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}} + C_{1\varepsilon} \frac{\varepsilon}{k} C_{3\varepsilon} G_b. \quad (6)$$

where  $G_k$  and  $G_b$  represent the generation of  $k$  by, respectively, mean velocity gradients and buoyancy,  $Y_M$  is the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate,  $\sigma_k$  and  $\sigma_\varepsilon$  are the turbulent Prandtl numbers for  $k$  and  $\varepsilon$  equal to 1 and 1.2,  $\nu$  is the kinematic viscosity.  $C_1$  is evaluated as function of the modulus of the mean rate of strain tensor,  $S$ .  $C_2$  and  $C_{1\varepsilon}$  are constants equal to 1.9 and 1.44, while  $C_{3\varepsilon}$  is calculated as function of the flow velocity components with respect to the gravitational vector. Realizable  $k$ - $\varepsilon$  model performance was compared against standard  $k$ - $\varepsilon$  model [10] and RNG  $k$ - $\varepsilon$  model [11]. However, the specifics of these two models are not presented as they are not a part of the CFD model under validation.

Combustion was modelled through the Eddy Dissipation Concept (EDC) [12]. The rate of reaction of the species  $i$  is evaluated as follow:

$$R_i = \frac{\rho(\xi^*)^2}{\tau^* \left[ 1 - (\xi^*)^3 \right]} (Y_i^* - Y_i), \quad (7)$$

$$\text{with } \xi^* = C_\xi \left( \frac{\nu \mathcal{E}}{k^2} \right)^{1/4} \text{ and } \tau^* = C_\tau \left( \frac{\nu}{\mathcal{E}} \right)^{1/2}$$

where  $Y_i$  is the species mass fraction, with value  $Y_i^*$  over the time scale  $\tau^*$ , which represents the fine structure regions residence time,  $\xi^*$  is the fine scale length and  $\nu$  is the kinematic viscosity.  $C_\xi$  and  $C_\tau$  are the volume fraction and times scale constants, equal to 2.1377 and 0.4082. The EDC model includes detailed chemical mechanisms. In the present model, 18 elementary reactions and 9 species are considered for hydrogen combustion in air. Complete description of chemical reaction mechanism is given in [13].

The DO model was employed to simulate radiation [14]. The Radiative Transfer Equation (RTE) is solved for a finite number of solid angles  $\Omega'$  associated to the direction  $\vec{s}$ :

$$\nabla \cdot (I(\vec{r}, \vec{s}) \vec{s}) + (\kappa + \sigma_s) I(\vec{r}, \vec{s}) = \kappa n^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(\vec{r}, \vec{s}') \Phi(\vec{s} \cdot \vec{s}') d\Omega' \quad (8)$$

where  $\kappa$  is the absorption coefficient,  $\sigma_s$  indicates the scattering coefficient and  $\vec{r}$  is the position vector in  $\vec{s}$  direction,  $n$  is the refractive index and  $\Phi$  is the scattering phase function. The direction  $\vec{s}$  of the control angle is determined by the polar and azimuthal angles, respectively  $\theta$  and  $\phi$ . The number of angular divisions for  $\theta$  and  $\phi$ , respectively  $N_\theta$  and  $N_\phi$ , can be increased to obtain a finer spatial discretization and more accurate calculation. The solid angle is furtherly subdivided in  $\theta$  and  $\phi$  pixels to take account of any control angle overhang. When the control volume face is not aligned to the global angular discretisation, control angles may be partially outgoing and partially incoming to the face. Pixelation subdivides each control angle in smaller portions where radiation can be treated as incoming or outgoing.

### 3.2 Modelling of release source

The operating pressure of the release in experimental tests is in the range 2-6 bar abs. At pressures above 2 bar abs an under-expanded jet is expected. The diameter of notional nozzle was calculated using Ulster's under-expanded jet theory [15], which assumes isentropic expansion, choked flow at the real nozzle, speed of sonic flow at the notional nozzle, and Abel-Noble equation of state (EOS) to describe the non-ideal behaviour of the gas. As the release is cryogenic, the problem must be handled carefully. The stagnation conditions are all located in the vapour/gas phase. During expansion, the saturation curve may be crossed leading to a multiphase release. However, even considering the worst-case scenario, i.e. lowest recorded temperature (48 K), highest pressure (6 bar) and isentropic expansion to ambient pressure, the resulting point will be in the gaseous phase. In the experiments, the lower temperatures (< 60K) are coupled to pressure equal to 2 bar, distancing the nozzle conditions from the saturation curve. The second consideration regards the validity of Abel-Noble EOS for cryogenic releases. Abel-Noble EOS was compared to NIST EOS [16], which is generally employed to model LH<sub>2</sub> releases [5]–[7]. Density comparisons for several pressures are shown in Figure 2. The deviation is negligible for the range of pressure under study (2-6 bar) while it becomes significant as the pressure increases. Thus, Abel-Noble EOS and the notional nozzle approach can be applied to the release cases under analysis.

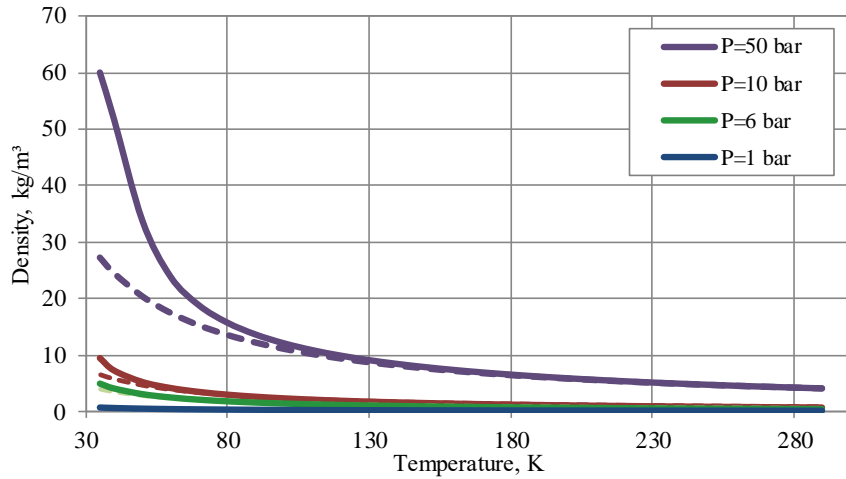


Figure 2. Effect of EOS on density evaluation: NIST (—) versus Abel Noble (--) equations

The calculated mass flow rate is compared against the entire set of experiments in Figure 3. 5 releases of the tests with orifice diameter equal to 1.25 mm were selected for the CFD study. The maximum deviation is about 10% and it is given for test 5. This discrepancy may be due to measurements uncertainty, as the measured mass flow rate is lower than a test with equal diameter and pressure but higher temperature ( $T=91$  K,  $\dot{m}=0.66$  g/s), while colder temperature should correspond to increase of released mass. The evaluated notional nozzle conditions are presented in Table 2.

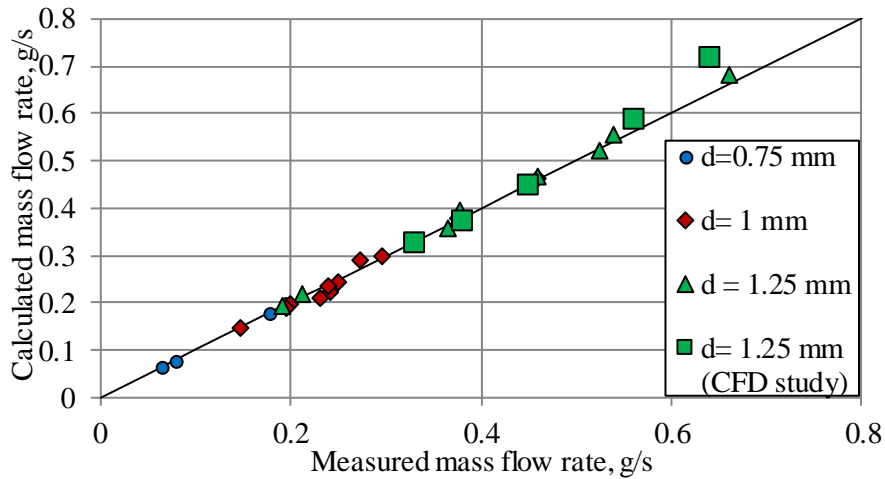


Figure 3. Calculated versus experimental mass flow rate

Table 2. Calculated notional nozzle conditions for the selected tests

| Test No. | Inlet temperature, K | Inlet velocity, m/s | Density, kg/m <sup>3</sup> | Notional diameter, mm | Calculated mass flow rate, g/s | Variation calculated mass flow rate from experiment, % |
|----------|----------------------|---------------------|----------------------------|-----------------------|--------------------------------|--|
| 1        | 53                   | 554.9               | 0.461                      | 1.27                  | 0.326                          | -1.26  |
| 2        | 40                   | 480.6               | 0.614                      | 1.27                  | 0.376                          | -1.10  |
| 3        | 63                   | 600.7               | 0.393                      | 1.56                  | 0.451                          | 0.25   |
| 4        | 65                   | 612.6               | 0.378                      | 1.80                  | 0.589                          | 4.93   |
| 5        | 68                   | 628.1               | 0.360                      | 2.01                  | 0.717                          | 10.78  |

### 3.3 Computational domain and grid

Given the axisymmetric nature of the problem, a quarter of the domain was considered for the analysis. Two calculation domains were used to perform simulations:

- Rectangular domain with dimensions 0.5 m x 0.5 m x 3 m. The hood geometry was not included. The aim of the analysis was the investigation of the free jet fire characteristics without the effect of facility geometry and exhaust hood volumetric flow rate.
- Rectangular domain with dimensions 1.2 m x 1.2 m x 2 m. The hood geometry was included in the numerical grid. In experiments, the hood was constituted by a bottom square section connected to a circular conduit for extracting the combustion fumes. In the present study the top part was assumed as square, considering the same section area as the circular duct. Figures 4a and 4b show a view of the domain and numerical grid.

The release source was approximated as square, with release area equal to the notional nozzle. As shown in Table 2, the 5 release tests resulted in 4 different notional nozzle diameters ( $D_{\text{eff}}$ ). Thus, 4 hexahedral numerical grids were created, adapting the release source and mesh to the test. The cell size varied from the notional nozzle size to about 10 cm in the far field. A grid independence study is presented in section 4.1.2. The grid refinement in proximity of the release point is shown in Figures 4c and 4d for the coarse and fine mesh respectively. The maximum expansion ratio was 1.1 in the nozzle proximity. The number of control volumes (CVs) in the calculation domain varied, e.g. 267317 CVs in test 1, and 211587 CVs in test 5 for the configuration including the hood geometry. The releases were treated as steady-state. The velocity and temperature evaluated at the notional nozzle and indicated in Table 2 were imposed as inlet conditions at the nozzle. The turbulent intensity (TI) and turbulent length scale (TLS) were imposed as  $TI=25\%$  and  $TLS=0.07D_{\text{eff}}$ , following the conclusions of the LES study on under-expanded hydrogen jet flame length and shape performed in [17].  $TLS=0.07D_{\text{eff}}$  is usually indicated for fully developed pipe flows [18]. The domain boundaries were modelled imposing a gauge pressure=0 and dry air was considered. However, section 4.1.5 analyses the case with moist air. The release pipe was assumed to be 10 cm long. The surface beneath the release pipe was modelled as non-slip adiabatic boundary. The radiometers, represented by 2x2 cm surfaces, were modelled as isothermal non-slip walls with emissivity 1. In this way, no radiation will be reflected by the surface and the received radiative heat flux will take account of the entire incident radiation. The only absorbing/emitting species in hydrogen combustion is water vapour. In this study, it was treated as a grey gas with Planck mean absorption coefficient defined as function of temperature and  $H_2O$  partial pressure. The function was determined from interpolation of Hubbard and Tien's data available in [19] and it will be indicated further in the text as HT. Scattering was not considered as it is negligible for combustion not involving soot. The Radiative Transfer Equation (RTE) was discretised using 5x5 angular divisions and 3x3 pixels, as suggested by [18]. The radiative discretisation will be varied in the range 5x5-15x15 angular divisions and 3x3-10x10 pixels in section 4.1.4. SIMPLE procedure was chosen for velocity-pressure coupling and convective terms were discretized using the second order upwind scheme. The stainless-steel hood walls considered in section 4.2 were modelled as non-slip walls with emissivity 0.6 [20]. The above described characteristics constitute the initial settings of the problem. Several parameters were varied in the proposed sensitive study and they will be indicated and discussed in the following sections.

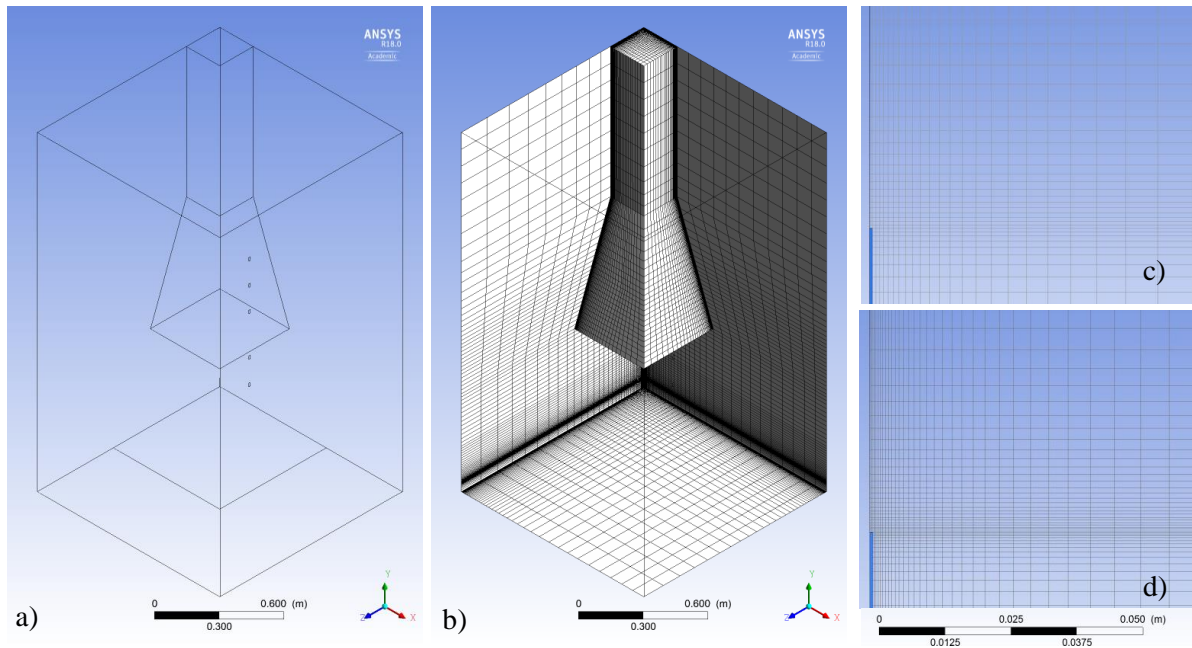


Figure 4. Numerical grid details: 3D isometric view of computational domain (a) and grid (b) with hood inclusion; detail of area in proximity of release for coarse mesh (c) and fine mesh (d) for grid sensitivity study

## 4 RESULTS AND DISCUSSION

The aim of this section is to analyse the effect of the modifications of a set of parameters on the simulated thermal radiation. The sensitivity study is presented for test 1, with the exception of section 4.2.3, where the results are shown for tests 4 and 5. The effect of each variation was investigated singularly and in sequence, selecting each time the best value/sub-model and applying it in the following part of the study. The effect of physical models and numerical features, such as the turbulence model and radiation discretisation, and grid refinement level were assessed for a free jet fire configuration, so that results of the parametric study would be free from further experimental uncertainty, such as the fumes velocity at the hood. Results are discussed in section 4.1. Analysis in section 4.2 includes the hood geometry, investigating the effect of the experimental settings, such as the exhaust gases extraction speed. Once the set-up of the model was completed, it was applied to the whole set of releases to validate it against experiments. Evaluations are shown in section 4.3.

### 4.1 Free jet fire

#### 4.1.1 Effect of turbulence model

Simulations were performed for the standard  $k-\varepsilon$ , RNG  $k-\varepsilon$  and realizable  $k-\varepsilon$  turbulence models. The resulting axial temperature distribution is reported in Figure 5, showing significant differences. Considering a 1300-1500 K region as corresponding to the visible flame length [21], the standard  $k-\varepsilon$ , RNG  $k-\varepsilon$  and realizable  $k-\varepsilon$  models resulted in flame length included in the range, respectively, 0.5-0.59 m, 0.38-0.44 m and 0.63-0.72 m. Experimental flame length, evaluated as average of visible and infrared recordings, resulted 0.66 m. The realizable  $k-\varepsilon$  turbulence model gives the best value compared to experiment. However, it must be highlighted that flame length evaluations in experiments and simulations are somehow arbitrary and uncertain, mining the reliability of results. The different temperature distribution affects strongly the radiative heat flux, shown in Figure 6, where the 5 diamonds of each curve represent the records at the 5 sensors. The realizable  $k-\varepsilon$  model shows the best agreement with experiment, although a significant underestimation of the radiative heat flux by approximately 50% for RD1.

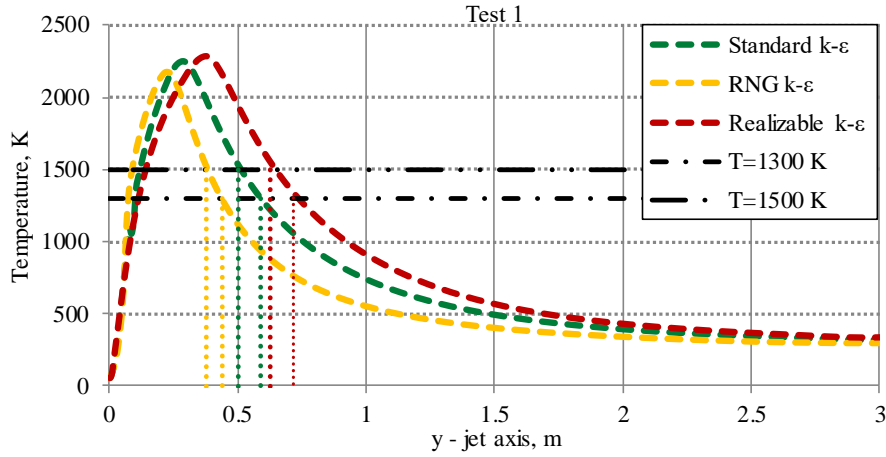


Figure 5. Effect of turbulence model on axial temperature distribution

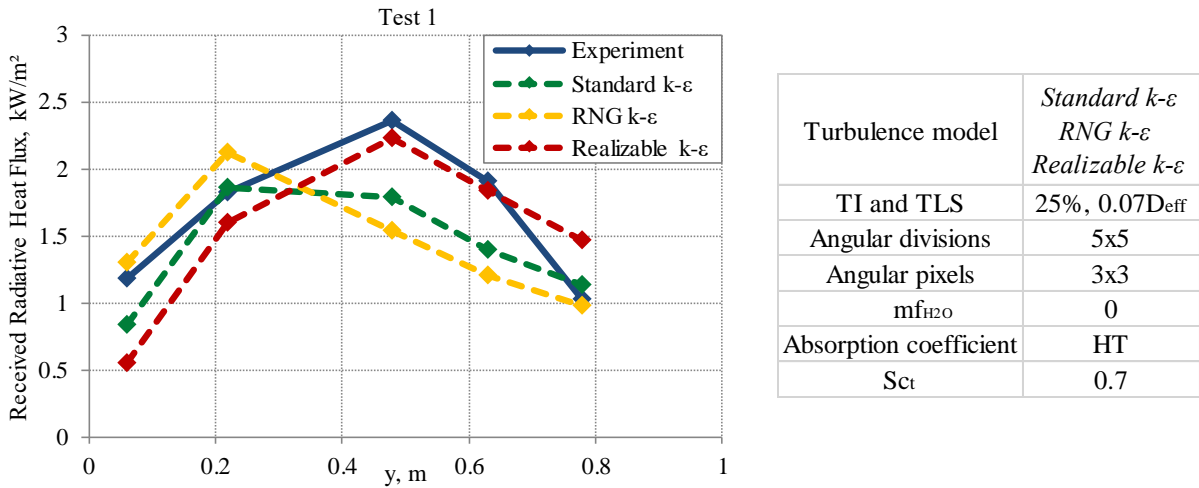


Figure 6. Effect of turbulence model on radiative heat flux

#### 4.1.2 Grid independency test

A sensitivity study on the computational domain resolution was conducted at the initial stage, in agreement with the CFD model evaluation protocol [22]. A finer mesh was created, heeding the regions where higher gradients and complex phenomena are expected. Thus, the length of the computational cells was halved where the release point, the jet flame and the radiation sensors are located. An expansion ratio equal to 1.1 was maintained. The total number of CVs was increased from 196314 to 507524. The effect on the axial temperature distribution was found to be negligible, while slight differences were observed on its radial distributions. Figure 7 shows the radial distributions of temperature and water vapour at 0.2 and 0.6 m from the release. The effect of the mesh refinement on the measured radiative heat flux is shown in Figure 8 and it is limited to the proximities of the release point, resulting in a maximum difference of 5% at sensors RD1 and RD2 ( $y=0.06$  and  $y=0.22$  m). Therefore, it is concluded that the built mesh using the minimum refinement (1 CV at the release point) can be used for the following analysis, as the mesh resolution is sufficient to solve accurately the problem.



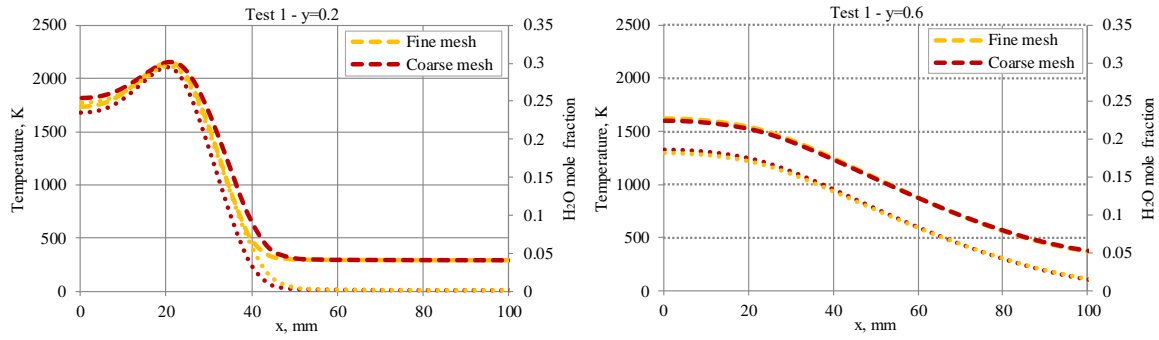


Figure 7. Results for grid independency: radial temperature (---) and H<sub>2</sub>O mole fraction (...) distributions at 0.2 and 0.6 m from the release

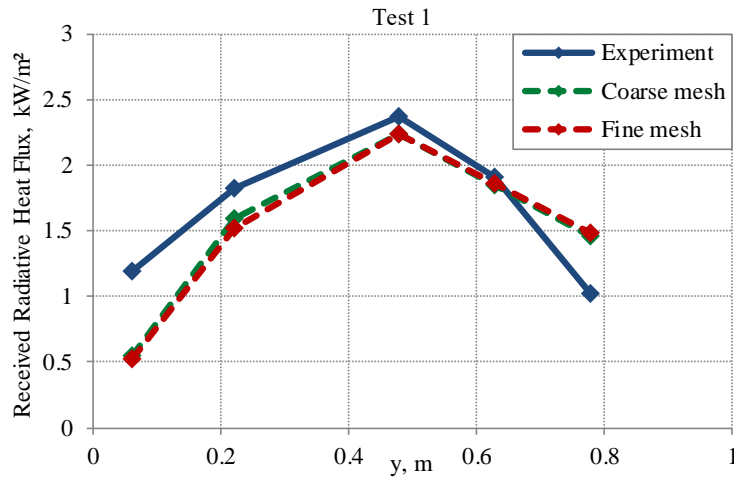
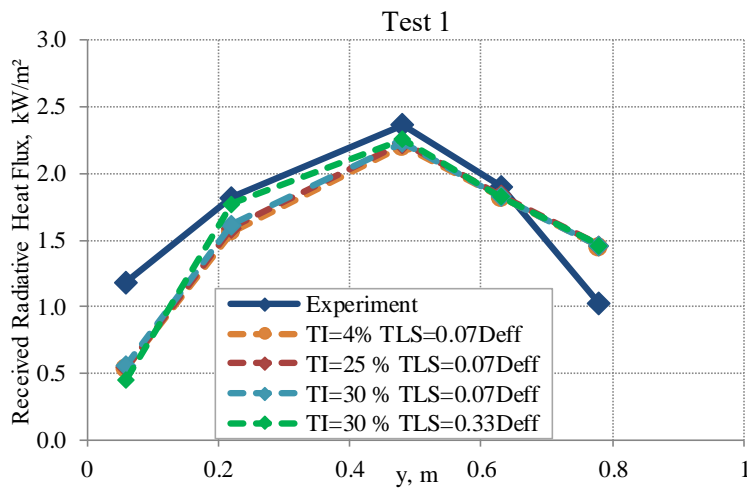


Figure 8. Results for grid independency: received radiative heat flux

#### 4.1.3 Effect of inlet turbulence intensity and turbulence length scale

The current section is aimed to define the appropriate turbulence quantities at the inlet flow, i.e. at the notional nozzle exit. Indeed, these parameters affect the mixing occurring between the fuel and oxidizer, influencing the flame shape and species distribution in the jet fire. The flow perturbations at the inlet were modelled in terms of turbulence intensity and turbulence length scale. The case employing  $TI=25\%$  and  $TLS=0.07 \cdot D_{eff}$  was compared to: a)  $TI=4\%$  and  $TLS=0.07 \cdot D_{eff}$ , based on experimental observations on air under-expanded jets [23]; b)  $TI=30\%$  and  $TLS=0.33 \cdot D_{eff}$ , based on the results of a parametric study conducted at HySAFER on hydrogen jet concentration decay. Figure 9 demonstrates that the turbulence inlet parameters affect the radiative heat flux only in proximity of the release point. However, the difference is negligible for turbulence intensity and turbulence length scale lower than, respectively,  $30\%$  and  $0.33 \cdot D_{eff}$ . The effect on flame length was limited to  $\pm 2$  cm variation. A further analysis was conducted for  $TI=30\%$  and  $TLS=0.07 \cdot D_{eff}$ . The similarity of the results to the cases with equal  $TLS$  and different  $TI$  indicate that  $TLS$  is the cause of the variation for  $30\%$  and  $0.33 \cdot D_{eff}$ . However, if for  $30\%$  and  $0.33 \cdot D_{eff}$  case the prediction improves for radiation sensor 2, it worsens for sensor 1. Therefore, the selected inlet conditions are turbulence intensity  $25\%$  and turbulence length scale  $0.07 \cdot D_{eff}$ .

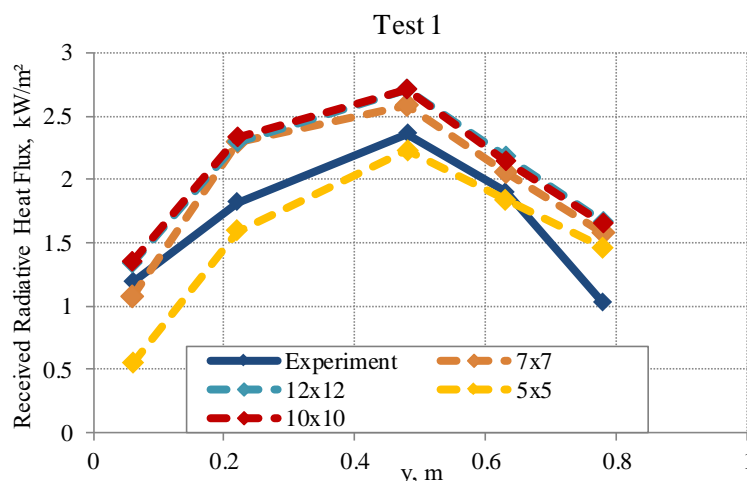


|                        |   |
|------------------------|---|
| Turbulence model       | Realizable k-ε  |
| TI and TLS             | 4%, 25%, 30%<br>0.07D <sub>eff</sub> , 0.33D <sub>eff</sub> |
| Angular divisions      | 5x5   |
| Angular pixels         | 3x3   |
| mf <sub>H2O</sub>      | 0   |
| Absorption coefficient | HT  |
| Sc <sub>t</sub>        | 0.7   |

Figure 9. Effect of inlet turbulent intensity and turbulent length scale

#### 4.1.4 Effect of radiation model angular discretisation

The number of Theta and Phi divisions determine the number of control angles associated to the RTE. 5x5 divisions are generally suggested for problems involving small geometry features and strong variation of temperature in space [18]. Under-prediction of radiative heat flux at the radiometers located in proximity of the release point may be due to insufficient angular discretisation, preventing the sensors to receive the radiation emitted by the flame along all its length. Thus, the number of divisions was increased, maintaining the same number of pixels. Comparisons for 5x5, 7x7, 10x10 and 12x12 are shown in Figure 10. Case with 15x15 was also analysed but not reported in Figure 10, as it practically overlaps the curves with 10x10 and 12x12 divisions. It was found that the angular discretisation has a great effect on the recorded radiative heat flux. Over 10x10 divisions the results are not sensitive to any further refinement. 10x10 was chosen as it is the adequate compromise between accuracy of the results and computational time (simulation time from 5x5 case increases by 1.9 for 10x10 and 2.4 for 12x12 angular divisions). Maximum deviation from experiment is given for sensor RD5 (about 40%).



|                        |                                  |
|------------------------|----------------------------------|
| Turbulence model       | Realizable k-ε                   |
| TI and TLS             | 25%, 0.07D <sub>eff</sub>        |
| Angular divisions      | 5x5, 7x7, 10x10,<br>12x12, 15x15 |
| Angular pixels         | 3x3, 10x10                       |
| mf <sub>H2O</sub>      | 0                                |
| Absorption coefficient | HT                               |
| Sc <sub>t</sub>        | 0.7                              |

Figure 10. Effect of number of angular divisions (3x3 pixels)

3x3 Theta and Phi pixels are usually suggested for problems involving symmetry [18]. The number of pixels was increased to 10x10 and no variation was sensed in the results. The reason may be due to the use of a rectilinear hexahedral mesh, where the control volumes faces are aligned to the angular

discretization, preventing the control angle overhang problem to arise. Thus, 3x3 pixels are sufficient to obtain reliable results and they were used with 10x10 angular divisions in the following analysis.

#### 4.1.5 Effect of air humidity

The initial assumption of dry air for a controlled laboratory environment may not be adequate and the effect of water vapour presence must be assessed. As described in section 3.3, water vapour behaves as an absorbing/emitting species. Absence of water vapour in air implies that all the radiation emitted by the flame reaches the radiometers. Conversely, if air is humid, radiation is absorbed along the path to sensors, causing a decrease of the recorded radiative heat flux. The amount of absorbed radiation depends on temperature and quantity of water vapour in air, which determine the value of absorption coefficient considered in the radiation model, and the travelled distance. The amount of water vapour in air is highly variable, depending on location and time. Mass fraction equal to 0.008 was assumed, according to the average meteorological data for SNL location, i.e. relative humidity equal to 74% and temperature 288 K [24]. As shown in Figure 11, the presence of water vapour has a significant effect on simulation results, remarking how indispensable is the availability of accurate description of various test conditions from experimentalists, including relative humidity. Sensors RD4 and RD5 are less affected, as they are located in proximity of the wider portion of the combustion products plume. In the following sections, moist air will be considered, as it is more realistic and it provides better agreement with experiments.

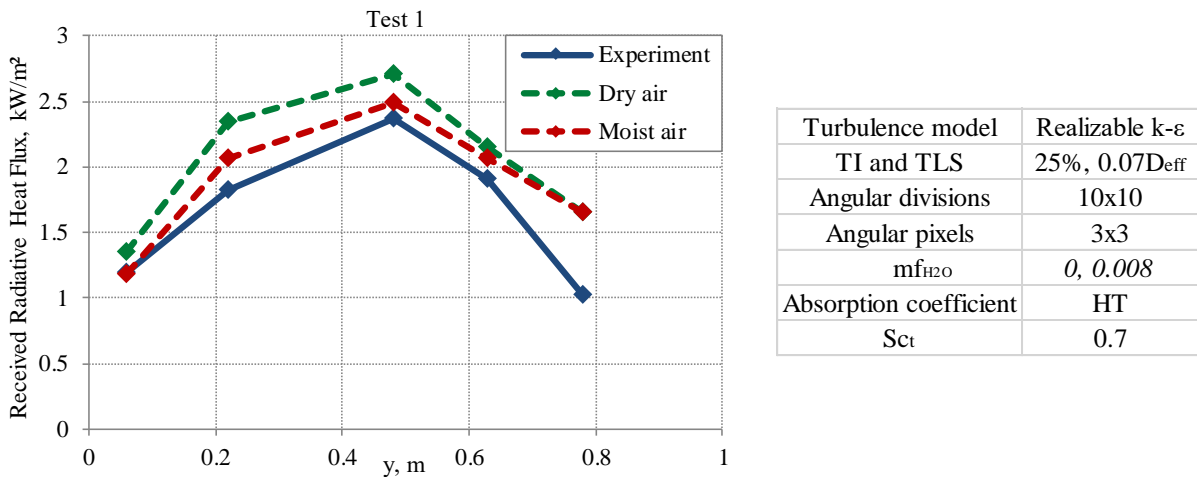
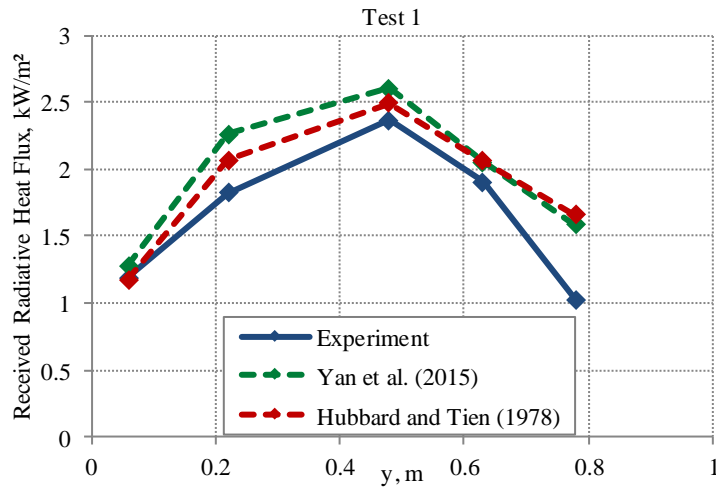


Figure 11. Effect of water vapour presence in air

#### 4.1.6 Effect of absorption coefficient

Hubbard and Tien's Planck mean absorption coefficient (HT) was compared to the coefficient evaluated according to Yan et al.'s (Y) calculations [25]. The two coefficients mainly differ for temperatures lower than 800 K, where HT coefficient is higher than Y coefficient. As shown in Figure 12, this difference is translated in less radiation at the sensors located close to the release point, as radiation from the flame has a longer distance to cover and, because of higher absorption coefficient, greater chance to be absorbed. Given the better agreement with experiments, HT formulation was selected for the model.

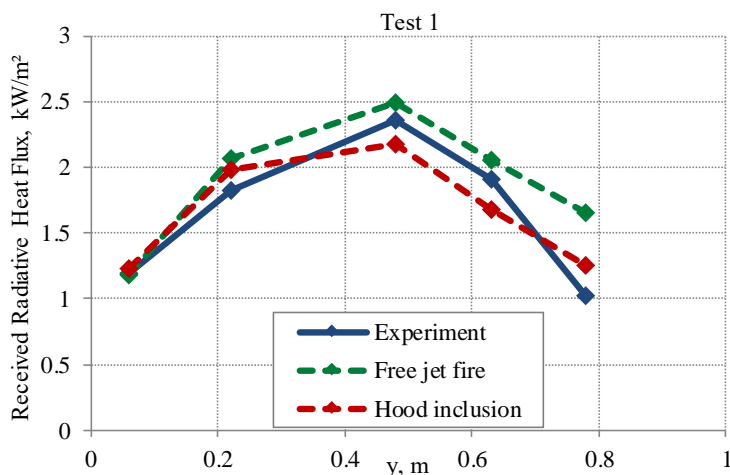


|                              |                           |
|------------------------------|---------------------------|
| Turbulence model             | Realizable k- $\epsilon$  |
| TI and TLS                   | 25%, 0.07D <sub>eff</sub> |
| Angular divisions            | 10x10                     |
| Angular pixels               | 3x3                       |
| mf <sub>H<sub>2</sub>O</sub> | 0.008                     |
| Absorption coefficient       | HT, Y                     |
| Sc <sub>t</sub>              | 0.7                       |

Figure 12. Effect of absorption coefficient

#### 4.2 Hood inclusion in the geometry

The laboratory was equipped with an exhaust gases system. Therefore, the combustion can be affected by the flow imposed at the hood. The extension of the computational domain including the hood was decided according to a sensitivity study on the domain size. The width of the domain was changed from 0.7 m to 1.2 m. Maximum variation of radiative heat flux of about 8% was detected on sensor RD1, leading to the choice of domain size=1.2 m. To ensure that the domain boundaries are located sufficiently far from the area of interest, an additional sensitivity analysis was conducted on the domain boundary conditions. Turbulence kinetic energy and turbulent dissipation rate were varied from, respectively,  $1.5 \cdot 10^{-4} \text{ m}^2/\text{s}^2$  and  $3.0 \cdot 10^{-6} \text{ m}^2$  (evaluated for the analysis in section 4.2) to unitary values. The effect on radiative heat flux was confined to 4% variation, which was considered acceptable considering the needs to minimize the impact of boundary conditions on simulation results and to limit the required computational time. Figure 13 shows the comparison between the results of the free jet fire and the configuration including the hood. The removal of the combustion products by forced ventilation caused a decrease of radiative heat flux, reaching over 30% reduction. A further observation shall be made on emissivity for the stainless steel of the hood, as it may vary in a wide range according to the material composition and the maintenance status. A parallel analysis, not shown in Figure 13, on the variation of the hood surfaces emissivity was conducted, varying it from 0.60 to 0.07 [20]. The maximum increase was +8% and it was detected on sensor RD5. Emissivity of 0.60 will be used in the following simulations.



|                              |                           |
|------------------------------|---------------------------|
| Turbulence model             | Realizable k- $\epsilon$  |
| TI and TLS                   | 25%, 0.07D <sub>eff</sub> |
| Angular divisions            | 10x10                     |
| Angular pixels               | 3x3                       |
| mf <sub>H<sub>2</sub>O</sub> | 0.008                     |
| Absorption coefficient       | HT                        |
| Sc <sub>t</sub>              | 0.7                       |
| V <sub>hood</sub>            | 7 m/s                     |

Figure 13. Effect of hood inclusion in the calculation domain (stainless steel emissivity=0.60)

#### 4.2.1 Effect of turbulent Schmidt number

The turbulent Schmidt number,  $Sc_t$ , was changed in the range 0.7-1. The variation affected the temperature and species distribution in the jet. Figure 14 shows that the increase of  $Sc_t$  causes the radiative heat flux from the first portion of the flame to decrease, while it has the opposite effect for the second half. The reason is due to the flame highest temperature region movement towards the flame tip, thus increasing the emitted radiation from the final part of the flame.  $Sc_t=0.9$  was selected for the following analysis, as it reproduced better the experimental radiative heat flux distribution trend, decreasing the gap between simulation and experiment for the sensors recording the highest radiative heat flux. In addition,  $Sc_t=0.9$  gave the best reproduction for axisymmetric jets in the review proposed by [26].

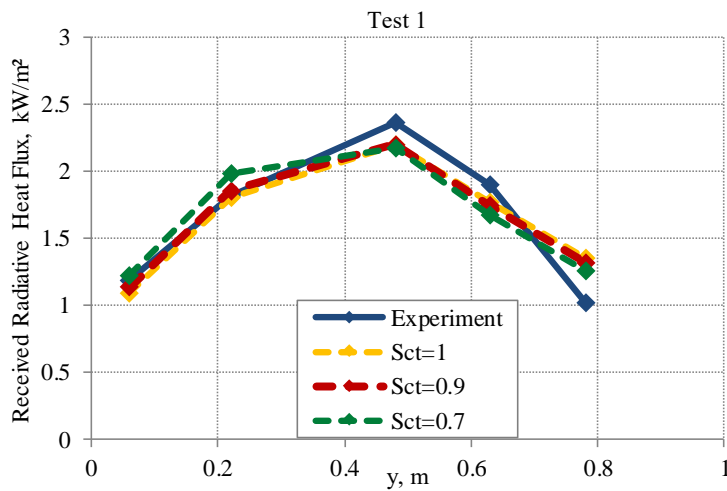


Figure 14. Effect of turbulent Schmidt number

|                        |                           |
|------------------------|---------------------------|
| Turbulence model       | Realizable k- $\epsilon$  |
| TI and TLS             | 25%, 0.07D <sub>eff</sub> |
| Angular divisions      | 10x10                     |
| Angular pixels         | 3x3                       |
| mf <sub>H2O</sub>      | 0.008                     |
| Absorption coefficient | HT                        |
| $Sc_t$                 | 0.7, 0.9, 1               |
| V <sub>hood</sub>      | 7 m/s                     |

#### 4.2.2 Effect of extraction velocity in the hood

For each test, the volumetric flow rate of the ventilation system was adapted to the released mass flow rate of hydrogen. The only available experimental data is the range of variation of the volumetric flow rate, 5100-7650 m<sup>3</sup>/h, corresponding to extraction velocity 7.0 m/s and 10.5 m/s respectively. No exact data for each test is available. Therefore, the minimum fumes speed has been considered in sections 4.2 and 4.2.1, based on the assumption that since the hydrogen mass flow rate (0.33 g/s) is closer to the minimum of the released mass range (about 0.1 g/s), the consequent extraction velocity will be more likely to be similar to the minimum of 7.0 m/s. However, tests 4 and 5 are characterised by a higher mass flow rate of 0.56-0.64 g/s, which is closer to the maximum mass flow rate of the overall tests set (0.7 g/s). Thus, fumes speed should be closer to 10.5 m/s rather than 7.0 m/s. This section aims to analyse the effect of the ventilation velocity on such releases, analysing the cases with minimum and maximum volumetric flow rate imposed at the hood as extreme cases. Figure 15 shows the effect of the hood extraction speed on the radiative heat flux. Since minimum and maximum limits were considered, the radiative heat flux curve simulating the actual fumes speed should be located between the green and red dashed curves, representing, respectively, the simulations for 7.0 and 10.5 m/s. For both the releases, considering the minimum extraction velocity led to a considerable overestimation (+36%) of the radiative heat flux for the sensors more exposed to the radiation from combustion products. The increase of the extraction velocity to the maximum limit, led to a reasonable reproduction of the experimental data, with deviations contained in the range  $\pm 14\%$ . Therefore, extraction velocity of 10.5 m/s is considered for tests 4-5, while 7.0 m/s is considered for releases 1-3.

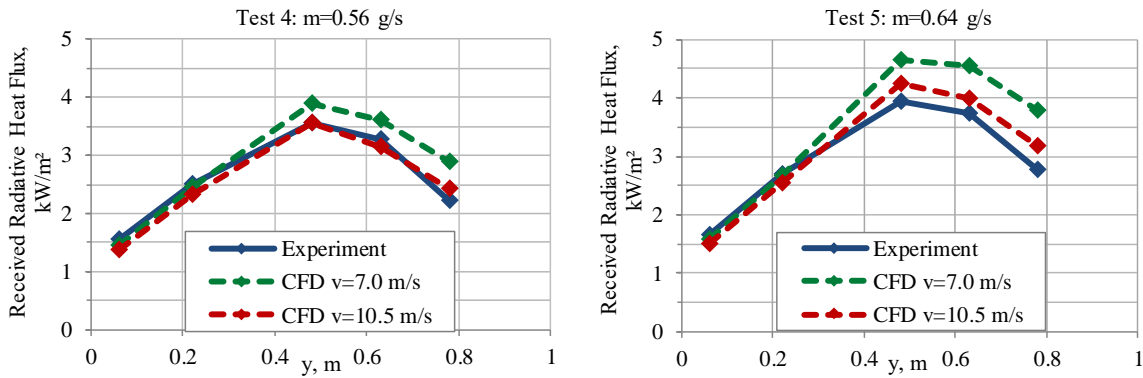


Figure 15. Effect of the hood extraction velocity in tests 4 and 5

#### 4.3 Definition of model set-up based on the parametric study and validation

Following the conclusions of the previous sections, the best settings for the predictive model were identified and they are summarized in Table 3.

Table 3. Model set-up

| Turbulence model                      | Realizable $k-\varepsilon$                          |
|---------------------------------------|---|
| Turbulence intensity and length scale | 25% and 0.07D                                       |
| Angular divisions                     | 10 x 10   |
| Angular pixels                        | 3 x 3   |
| Water vapour mass fraction            | 0.008   |
| Absorption coefficient                | Hubbard and Tien (1978)                             |
| Turbulent Schmidt number              | 0.9   |
| Velocity at the hood                  | Tests 1,2,3: $v=7.0$ m/s<br>Tests 4,5: $v=10.5$ m/s |

Results for the 5 tests are shown in Figure 16. Experimental radiative heat flux is predicted in simulations within  $\pm 15\%$ , which is acceptable for safety engineering design accuracy. There is one exception, i.e. the overestimations of flux at 5<sup>th</sup> sensor for tests 1 and 2, where radiation is 29% and 17.5% higher respectively. It must be reminded that this sensor is the most affected by the hood characteristics taken in simulations, such as the material emissivity or the hood geometry, which is entirely approximated as square. In addition, the 5<sup>th</sup> sensor is the most exposed to the water vapour of the jet flame, strongly affected by the velocity field imposed by the extraction system. Since no precise volumetric flow rate was available for each test, the assumption of either minimum or maximum flow velocity in the hood can lead to inaccuracy of results. The water vapour, while accumulating and cooling down, may also be affected by condensation, which is not taken in account in simulation. Experimental data on relative humidity were not available. Thus, the annual average for California (74%) was accepted. However, relative humidity is generally lower in environments where controlled air ventilation systems are present, such as combustion or chemical laboratories. Therefore, the slight under predicting trend present in most of the tests might be caused by such approximation.

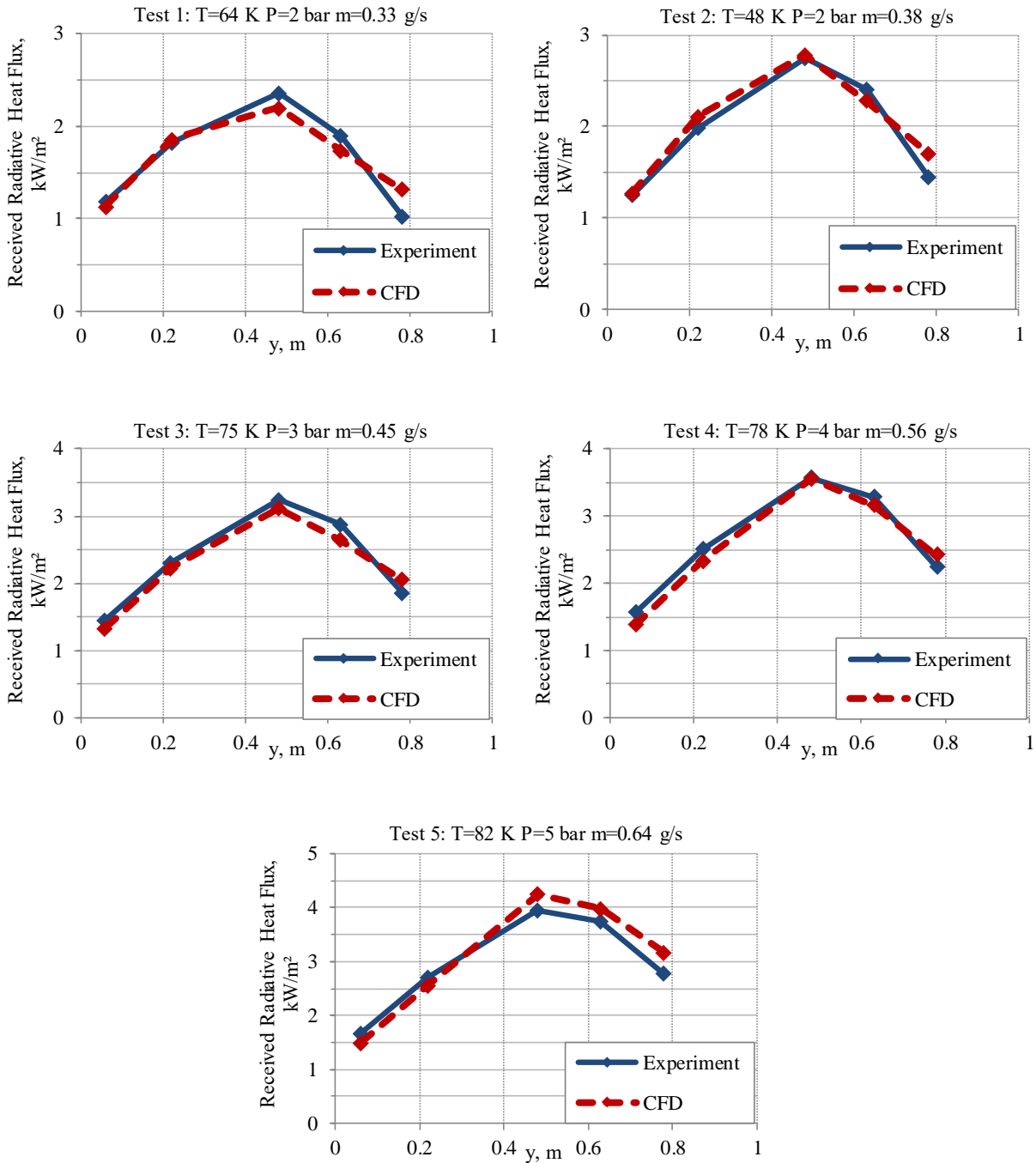


Figure 16. Radiative heat flux evaluation for validation experiments (model set-up: Table 3)

Table 4 reports the flame length evaluations based on the range of temperature 1300-1500 K and OH mole fraction= $10^{-3}$ . In general, the simulated flame length resulted somewhat longer than reported by experimentalists. The difference becomes more significant for jet fires in tests 4 and 5. This can be due to the mass flow rate overestimations in simulations by, respectively, 5% and 10% of the release source modelling (Table 2). Similarly, overpredictions were expected for the radiative heat flux, mainly for test 5. However, the maximum deviation was 14%, maintaining an acceptable accuracy of the results.

Table 4. Experimental and calculated flame length

| Test No.                        | 1    | 2    | 3    | 4    | 5    |
|---------------------------------|------|------|------|------|------|
| Experiment, m                   | 0.66 | 0.7  | 0.72 | 0.74 | 0.78 |
| CFD 1300 K, m                   | 0.74 | 0.80 | 0.85 | 0.94 | 1.02 |
| CFD 1500 K, m                   | 0.65 | 0.70 | 0.74 | 0.82 | 0.88 |
| CFD $m\dot{f}_{OH} = 0.001$ , m | 0.67 | 0.76 | 0.78 | 0.88 | 0.94 |

## 5 CONCLUSIONS

Simulations of cryogenic hydrogen jet fires were conducted to develop a predictive CFD model for assessment of thermal hazards. The simulations were validated against experiments in the range of pressures 2-5 bar abs and temperatures 48-82K. Release source was modelled using the notional nozzle theory [15]. Three turbulence models were compared and realizable  $k-\epsilon$  model showed the best agreement with the measured flame length and radiative heat flux. A sensitivity analysis of different parameters in simulations on thermal radiation from the jet fires has been carried out. The angular divisions' refinement for radiation model and humidity in air are shown to affect considerably the simulated radiative heat flux. 10x10 angular divisions' number was found to be the resolution, which provides independence of simulations on further refinement, for the problem under study. The presence of water vapour in air demonstrated a strong effect on the flame thermal radiation, causing variations up to 13%. Larger variations were found for different velocities at the hood for releases with higher hydrogen mass flow rate. Therefore, it is fundamental for experimental studies to make available exact measurements of test conditions to develop and validate predictive CFD models. The hydrogen inlet turbulence parameters, the absorption coefficient and turbulent Schmidt number showed to have a minor effect on radiative quantities. Turbulence intensity of 25% and turbulent length scale of  $0.07 \cdot D_{eff}$  at the inlet, Hubbard and Tien's absorption coefficient model and  $Sc_t=0.9$  were selected to describe the jet fires. Five cryogenic jet fire tests were used to validate the CFD model. For all five tests experimental radiative heat flux at 5 sensors along the jet flame was predicted within  $\pm 15\%$  accuracy, with few exceptions. During the study, the Abel Noble EOS was found to be applicable to cryogenic releases only for low pressure ( $< 6$  bar). Further research should be conducted to extend the domain of the CFD model applicability to high pressure cryogenic releases.

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