



Advanced Numerical Evaluation of the Jet Fire Caused by Accidental Releases of Liquid Hydrogen

Gianmaria Pio, Ernesto Salzano, Alessandro Tugnoli*

LISES – Laboratory of Industrial Safety and Environmental Sustainability, Department of Civil, Chemical, Environmental and Materials Engineering, University of Bologna, Via Terracini 28, 40131, Bologna, Italy
a.tugnoli@unibo.it

Considering the ongoing energy transition and the role of hydrogen within the process, a complete and comprehensive understanding of the safety aspects of hydrogen storage technologies is paramount to guarantee the sustainable development of these alternative solutions at an industrial scale. Among the available storage conditions, the possibility of using cryogenic temperatures to liquefy hydrogen has become more credible also due to the knowledge gained by the use of liquefied natural gas. Nevertheless, the peculiar properties of hydrogen promote dedicated analysis of the safety aspects. For these reasons, the current work presents an advanced numerical investigation on the jet fires deriving from the accidental release of liquid hydrogen, performed employing the open-source software Open Field Operation and Manipulation (OpenFOAM). Considering the dearth of experimental data at the boundary conditions of interest, preliminary investigations were carried out to assess the suitability of the existing sub-models and parameters for the evaluation of hydrogen jet fire caused by an accidental release from high pressure and atmospheric temperature. A maximum temperature of ~ 2300 K was observed within the core of the flame. The locations where the maximum temperatures were observed are in line with experimental data available in the current literature, confirming the validity of the implemented models for the evaluation of near-field fluid dynamics and overall chemistry. In addition, the case of a non-ignited release was also analyzed in terms of temporal and spatial profiles of temperature and hydrogen content within the numerical domain. Based on the gathered information, the maximum distance between the releasing point and the edge of the flammable cloud was obtained as a function of the releasing conditions. In conclusion, the availability of robust and validated models for the characterization of the accidental releases of liquid hydrogen paves the way for further development and wider adoption of this technology as well as the optimized design of mitigation systems and safety procedures.

1. Introduction

The use of hydrogen as a possible energy carrier has been largely and unquestionably promoted during the last decades. The physical properties of this species impose the utilization of extreme conditions for an economically convenient and sustainable transportation system (Zanobetti et al., 2023a). Among the others, cryogenic conditions have emerged as a solution of significant scientific and technological interest due to their unique properties and features allowing for economically convenient hydrogen transportation on an industrial scale (Raucci et al., 2015). However, the adoption of technologies based on liquid hydrogen (LH_2) or cryo-compressed hydrogen (CCH_2) poses new challenges in terms of safety aspects because of the elevated complexity of the interactions between storage cryogenic fluids and tanks as well as the limited readiness level of suitable protocols for handling and mitigation procedures (Cirrone et al., 2023)(Zanobetti et al., 2023b). In the circumstance of an accidental release, LH_2 and CCH_2 can generate jet fires if a suitable ignition source is present in the proximity of the releasing point (Cirrone et al., 2018). In this case, the evaluation of flame geometry and temperature distribution is essential (Gómez-Mares et al., 2009) as well as the quantification of ignitability and flame intensity (De Liso et al., 2024), especially for the evaluation of consequences and the assessment of the possibility of domino effects (Gómez-Mares et al., 2008). A typical approach for the characterization of flame geometry is the distinction of chemical phenomena from turbulence in dedicated studies. The former can be

focused on the estimation of the overall reactivity (e.g., in terms of the laminar burning velocity) through detailed kinetic mechanisms (Pio et al., 2022), whereas the latter is based on the development and implementation of dedicated models (Johansen, 2011). In this sense, it is worth mentioning that the hydrogen-air mixtures exhibit a fast overall reactivity also in the case of low initial temperatures, laminar, conditions, and atmospheric pressure (Pio and Salzano, 2018). On the one hand, the elevated reactivity of hydrogen together with the intense turbulence generated in the case of continuous release and the peculiar storage conditions make the application of the existing correlations and the numerical representation of the resulting scenario challenging (Vianello et al., 2020), promoting the use of computational fluid dynamic (CFD) for accurate representation of accidental scenarios of interest. On the other hand, in the proximity of the releasing point, under-expanded jets undergo a rapid expansion with the possible production of shock waves and characteristic flow structures known as Mach disks, as extensively documented in the literature (Panda and Hecht, 2017). The complexity of these phenomena makes the application of advanced numerical methods for the representation of near-field behavior impractical. Therefore, this limitation necessitates the adoption of simplified approaches to mimic the near-field behavior such as the notional nozzle, i.e., a hypothetical surface parallel to and larger than the real releasing section is placed where the flow reaches atmospheric pressure. The main properties of the flow at the notional nozzle are calculated under the assumption of an isentropic expansion. Consequently, the notional nozzle concept can be intended as a surrogate for the real release, defining the boundary conditions to be implemented in advanced computational analyses devoted to the characterization of under-expanded jets. The combination of notional nozzle and CFD approaches has been largely used in the literature for the characterization of the accidental release of under-expanded flammable jets (Cirrone et al., 2018). For these reasons, this work presents a numerical study aiming at the characterization of an accidental release of hydrogen by means of a combined strategy integrating CFD analysis with the notional nozzle concept. Because of the numerical nature of the implemented strategy and the lack of a robust dataset suitable for the validation at cryogenic conditions, the accuracy and robustness of the obtained results will be assessed through a comparison against experimental data, when available in the current literature. Indeed, considering the dearth of experimental data for validation purposes, preliminary investigations on the release of compressed gaseous hydrogen will be presented.

2. Methodology

In this work, a computational fluid dynamic (CFD) study was carried out employing Open Field Operation and Manipulation (OpenFOAM) to characterize the temporal and spatial distribution of temperature and composition in the proximity of an accidental release of hydrogen. The numerical investigation performed in this work is based on a cubic domain with dimensions 6 m x 3 m x 3 m that was discretized for numerical analysis. To balance computational efficiency and accuracy, an adaptive meshing approach was employed. More specifically, the mesh was refined in areas with rapidly changing physical properties, i.e., in the proximity of the releasing point, and coarser discretization was used in regions characterized by smoother variations. The implemented grid was selected based on a grid sensitivity analysis aiming at ensuring that reliable and not overly dependent on the specific mesh adopted results were obtained. The hydrogen inlet was located at the center of a lateral surface, 1.5 meters above the ground. The notional nozzle concept (Papanikolaou et al., 2012) was considered to assess the boundary conditions (i.e., notional nozzle size, temperature, and pressure) at the hydrogen inlet, considering a storage condition of 450 bar and a releasing hole having a diameter of 1 mm, at first. The abovementioned boundary conditions as well as NASA polynomial coefficients for the evaluation of thermodynamic properties were posed in agreement with experimental data available in the current literature and adopted for the sake of validation (Carboni et al., 2022). At a later stage, simulations were performed assuming lower pressures and temperatures as storage conditions, as reported in Table 1.

Table 1: Initial conditions considered for the numerical characterization of an accidental release of hydrogen in the atmosphere.

Case ID #	Pressure [bar]	Temperature [K]	Nozzle diameter [mm]
0	450	298	5
1	2	22	50
2	5	27	50
3	10	31	5
4	10	31	11.2
5	10	31	50

To provide sufficient elements for an effective and robust evaluation of the effects of the initial temperature on the flame structure and consequences of an accidental release of hydrogen, an additional case was considered having the initial pressure and nozzle diameter of Case ID #1, but an initial temperature of 100 K. For the sake of conciseness, this additional case was referred to as Case ID #1*. Regardless of the releasing conditions, the atmosphere within the domain is assumed a quiescent air with a uniform temperature of 298 K at the beginning of the simulation. The model incorporates mass and heat transfer throughout the domain and across all boundaries except the bottom surface, which represents the ground since no-slip and adiabatic boundary conditions were applied in that case. The sub-model *hePsiThermo* was considered to account for the specific enthalpy and compressibility, whereas transport coefficients were estimated through Sutherland's law. Large Eddy Simulation (LES) was adopted to optimize the estimation quality and computational cost, following the recommendations available in the current literature (Favrin et al., 2018). The Eddy Dissipation Concept (EDC) was implemented to combine kinetic mechanisms and turbulent mixing models in the evaluation of the chemistry of the system. The chemical reaction rate was estimated by using a modified Arrhenius equation and coefficients for the overall hydrogen combustion reaction available in the current literature (Marinov et al., 1996), as reported in Eq(1). To provide the ignition source, an element having a defined volume of 10 cm³ located on the symmetric axes with the releasing point was set at a temperature of 1200 K for 1 ms once a stable fluid dynamic regime was reached by a non-ignited jet.

$$k = A \cdot T^n \cdot e^{-\frac{E_a}{R \cdot T}} = 1.734 \cdot 10^5 \cdot T^{1.51} \cdot e^{-\frac{1726}{T}} \quad (1)$$

The spatial and temporal evolutions of the temperature, pressure, velocity, and gaseous composition within the numerical domain were estimated and compared with experimental data from the literature, when available.

3. Results and discussion

Figure 1 presents the spatial distribution of the estimated temperature, as obtained for Case ID #0. To evaluate also its evolution over time, two different instants are reported: 2.5 s and 3.5 s after the release, i.e., 0.5 s and 1.5 s after the introduction of an ignition source.

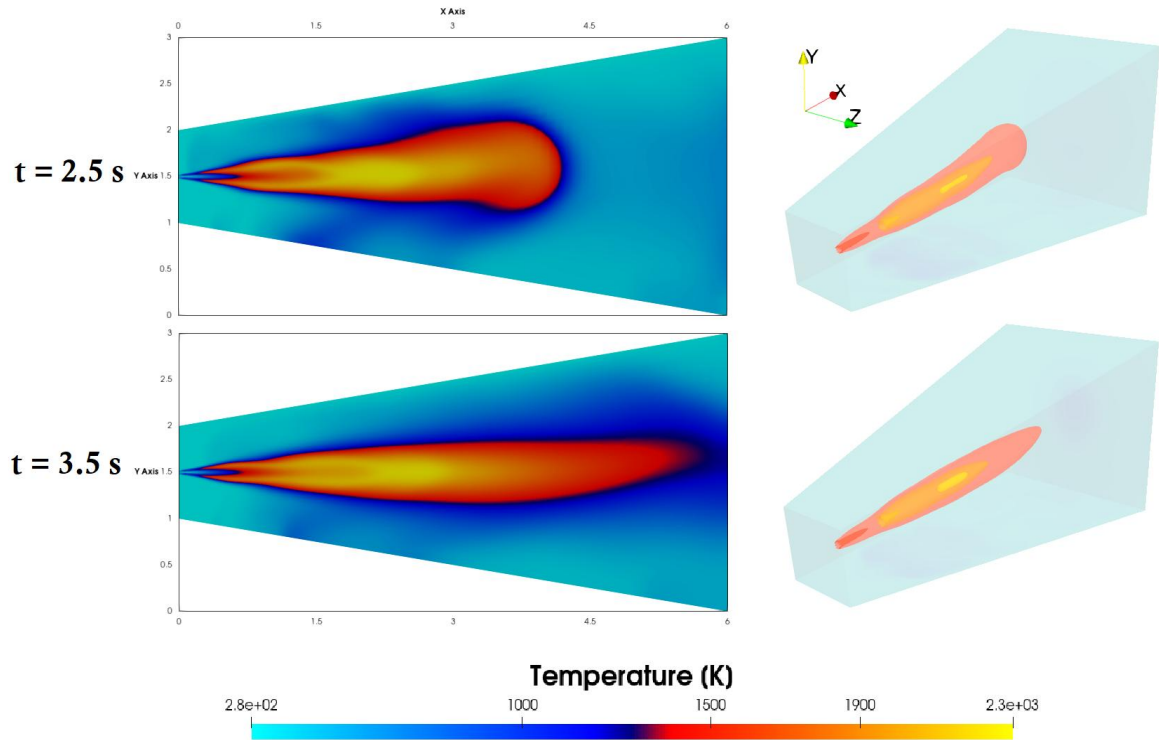


Figure 1: Estimated temperature distribution for Case ID #0, as obtained 0.5 s and 1.5 s after the ignition.

Although a tendency to slightly underestimate the buoyancy effects on the exhaust gas can be observed, a maximum temperature of 2307 K was estimated at 2.5 m from the releasing point. These values (i.e., estimated temperature and location) align with experimental measurements collected under comparable boundary conditions and reported in the current literature (Carboni et al., 2022). For these reasons, the implemented numerical structure was adopted for the analysis of cold-release, as well. Figure 2 reports the estimated temperature distribution as obtained for Case ID #1 and Case ID #1* 0.5 seconds after the ignition.

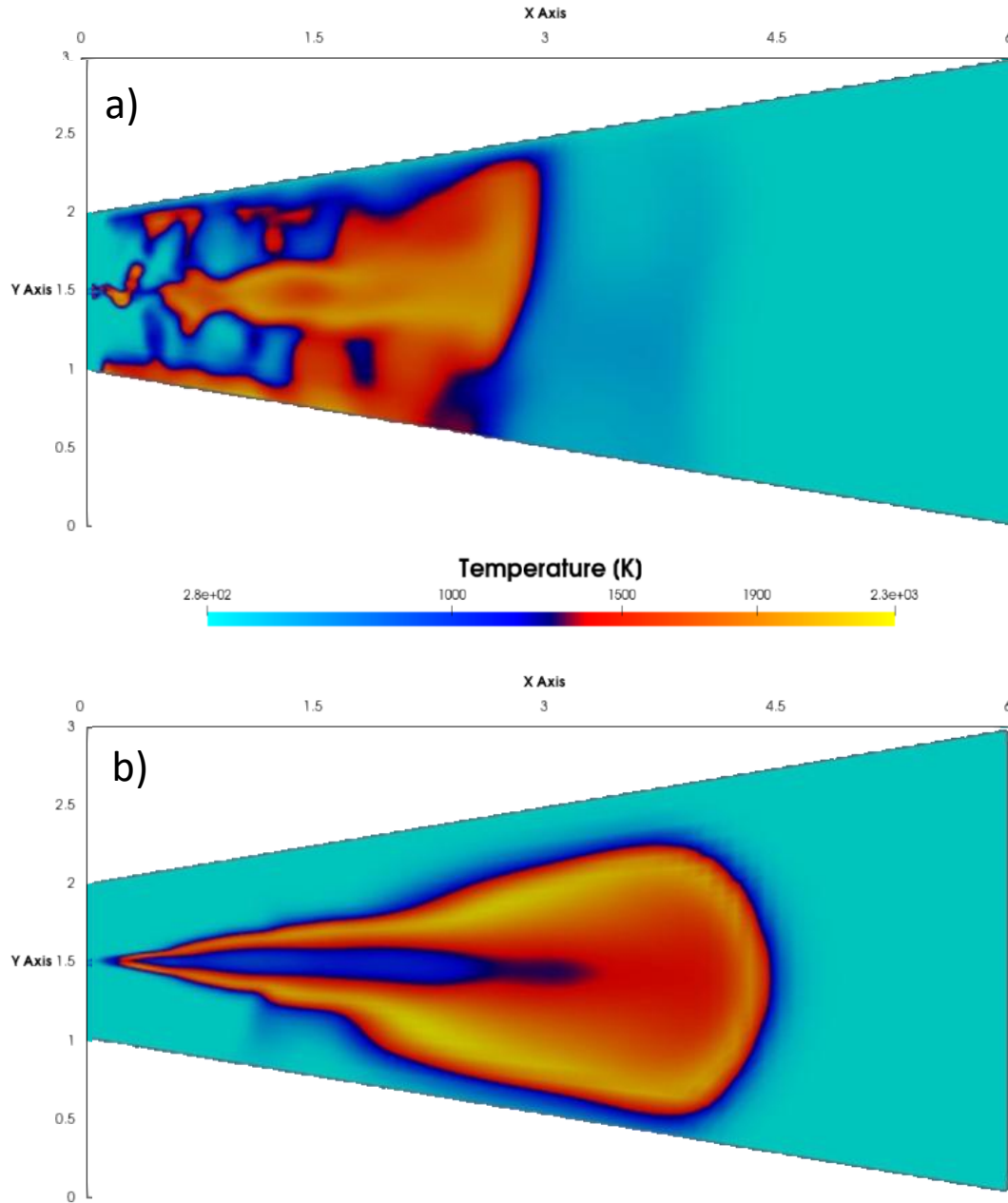


Figure 2. Estimated temperature distribution for Case ID #1 (a) and Case ID #1* (b), as obtained 0.5 s after the ignition.

While both Case ID #1* and Case ID #0 exhibit comparable lift-off distances and maximum temperatures, a distinct flame structure emerges. This is particularly remarkable especially if the diameter of the releasing nozzle is considered, namely 5 mm for Case ID #0 and 50 mm for Case ID #1*. Indeed, the nozzle diameter has been largely indicated as a determining parameter of the lift-off distances for the case of high-pressure release at atmospheric temperatures (Imamura et al., 2008). In addition, Case ID #1* displays a cooler, hydrogen-rich core extending approximately 3.5 m horizontally from the release point. This region, characterized by lower

temperatures and a higher hydrogen-to-oxygen ratio, suggests incomplete combustion, possibly due to poor mixing of the initial jet with the surrounding environment. This assumption is confirmed by the spatial distribution of velocity obtained from this simulation, indicating that the cold region is also dominated by the initial momentum. In contrast, Case ID #1* exhibits a wider, hot region, particularly near the ground. Notably, the maximum temperature in Case ID #1* is observed closer to the outer layer of the flame, likely due to localized oxygen deprivation, which can occur in regions with incomplete mixing of fuel and oxidizer.

Once Case ID #1 and Case ID #1* are compared, it is worth noting that the introduction of cryogenic conditions leads to significant differences in flame behavior even if similar setups and boundary conditions are employed. Notably, Case ID #1 exhibits lower lift-off distances (-50 %) than Case ID #1*, indicating a more rapid flame stabilization process. This can be also attributed to the different physical properties of the released mixtures, affecting the size of the momentum-dominated region. The lower initial temperature in Case ID #1 results also in unstable flame propagation and intense back-mixing phenomena, especially in the proximity of the release point. This phenomenon, characterized by the recirculation of hot combustion products back into the computational domain, can lead to enhanced mixing and potentially increased reaction rates in that area. In this sense, the enhanced combustion efficiency can be also a factor influencing the lift-off of the flame. Additionally, a distinct, partially separated, and stratified flame is observed in Case ID #1, only. This flame can be originated from an initial spread of cold hydrogen acting as a dense vapor. Similar conclusions on the flame structures can be drawn from the evaluation of the temperature distribution at 0.5 s after the ignition for the other analyzed cases. For the sake of conciseness and clarity, the obtained values for Case ID #2 are reported in Figure 3, exclusively.

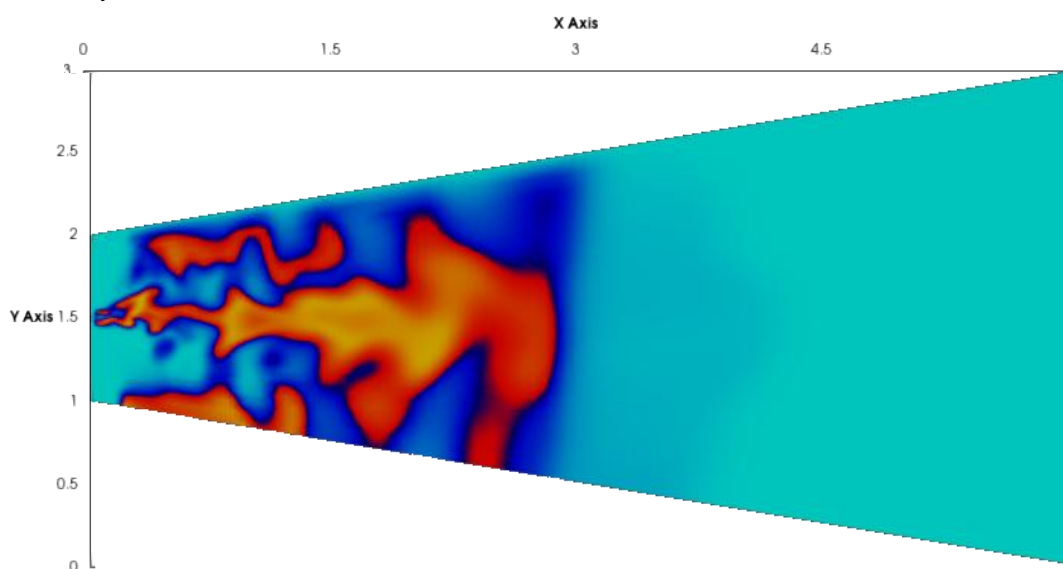


Figure 3 Estimated temperature distribution for Case ID #3 as obtained 0.5 s after the ignition.

The formation of a stratified flame structure is confirmed for all the investigated conditions assuming an accidental release from cryogenic conditions. This structure can significantly impact the overall combustion process, including flame stability, heat release rate, and pollutant emissions. Nevertheless, negligible variations can be observed in terms of the maximum temperature estimated within each test.

Based on the collected data, the implementation of lower initial temperatures leads to a significant reduction of the footprint of the flame resulting from an accidental release of hydrogen, because of the modified reactivity and physical properties of vapor. Therefore, the use of suitable models is necessary for a correct and accurate evaluation of the consequences associated with the jet fire scenarios, avoiding the use of over-conservative approaches on the safe side.

4. Conclusions

This work presents a numerical analysis aiming at the characterization of an accidental release of cryogenic hydrogen in the atmosphere. A computational fluid dynamic study employing the open-source software OpenFOAM was carried out to this scope. Different initial conditions as well as releasing sizes were tested, comparing numerical predictions with experimental data from the current literature, if available. The notional nozzle concept was employed for the assessment of boundary conditions to be adopted in advanced numerical studies. The temporal and spatial distributions of the main physical and chemical properties (e.g., temperature,

gaseous composition, pressure, and velocity) were monitored. A preliminary investigation considering a compressed gaseous hydrogen storage system was performed for the sake of validation of the numerical models adopted, because of the presence of a robust and comprehensive database for experimental measurements, showing a good agreement either in terms of temperature profiles or flame geometry. Afterward, cryogenic initial temperatures and moderate initial pressures (i.e., up to 10 bar) were analyzed, enlightening the effects of the boundary conditions on the flame lift-off and structure.

Acknowledgments

The authors gratefully acknowledge the financial support of the ELVHYS project, supported by the Clean Hydrogen Partnership and its members, funded by the European Union's Horizon Europe research and innovation program under grant agreement No 101101381.

References

- Carboni, M., Pio, G., Mocellin, P., Pilo, F., Vianello, C., Russo, P., Maschio, G., Salzano, E., 2022. Experimental and numerical characterization of hydrogen jet fires. *Int. J. Hydrogen Energy* 47, 21883–21896. <https://doi.org/10.1016/j.ijhydene.2022.05.010>
- Cirrone, D., Makarov, D., Molkov, V., 2023. Rethinking “BLEVE explosion” after liquid hydrogen storage tank rupture in a fire. *Int. J. Hydrogen Energy* 48, 8716–8730. <https://doi.org/10.1016/j.ijhydene.2022.09.114>
- Cirrone, D.M.C., Makarov, D., Molkov, V., 2018. Thermal radiation from cryogenic hydrogen jet fires. *Int. J. Hydrogen Energy* 1–12. <https://doi.org/10.1016/j.ijhydene.2018.08.107>
- De Liso, B.A., Pio, G., Salzano, E., 2024. Fire behaviour of liquid solvents for energy storage applications. *Process Saf. Environ. Prot.* 188, 726–734. <https://doi.org/10.1016/j.psep.2024.05.153>
- Favrin, S., Busini, V., Rota, R., Derudi, M., 2018. Practical LES modelling of jet fires: Issues and challenges. *Chem. Eng. Trans.* 67, 259–264. <https://doi.org/10.3303/CET1867044>
- Gómez-Mares, M., Muñoz, M., Casal, J., 2009. Axial temperature distribution in vertical jet fires. *J. Hazard. Mater.* 172, 54–60. <https://doi.org/10.1016/j.jhazmat.2009.06.136>
- Gómez-Mares, M., Zárate, L., Casal, J., 2008. Jet fires and the domino effect. *Fire Saf. J.* 43, 583–588. <https://doi.org/10.1016/j.firesaf.2008.01.002>
- Imamura, T., Hamada, S., Mogi, T., Wada, Y., Horiguchi, S., Miyake, A., Ogawa, T., 2008. Experimental investigation on the thermal properties of hydrogen jet flame and hot currents in the downstream region. *Int. J. Hydrogen Energy* 33, 3426–3435. <https://doi.org/10.1016/j.ijhydene.2008.03.063>
- Johansen, D., 2011. Implementation of Improved EDC Combustion Model in the Open LES Code FDS 213.
- Marinov, N.M., Westbrook, C.K., Pitz, W.J., 1996. Detailed and global chemical kinetics model for hydrogen. *Proc. Eighth Int. Symp. Transp. Phenom. Combust.* 1, 118–129.
- Panda, P.P., Hecht, E.S., 2017. Ignition and flame characteristics of cryogenic hydrogen releases. *Int. J. Hydrogen Energy*. <https://doi.org/10.1016/j.ijhydene.2016.08.051>
- Papanikolaou, E., Baraldi, D., Kuznetsov, M., Venetsanos, A., 2012. Evaluation of notional nozzle approaches for CFD simulations of free-shear under-expanded hydrogen jets. *Int. J. Hydrogen Energy* 37, 18563–18574. <https://doi.org/10.1016/j.ijhydene.2012.09.135>
- Pio, G., Dong, X., Salzano, E., Green, W.H., 2022. Automatically generated model for light alkene combustion. *Combust. Flame* 241, 112080. <https://doi.org/10.1016/j.combustflame.2022.112080>
- Pio, G., Salzano, E., 2018. Laminar Burning Velocity of Methane, Hydrogen and Their Mixtures at Extremely Low Temperature Conditions. *Energy & Fuels* 32, 8830–8836. <https://doi.org/10.1021/acs.energyfuels.8b01796>
- Raucci, C., Calleya, J., Suarez de la Fuente, S., Pawling, R., 2015. Hydrogen on board ship: A first analysis of key parameters and implications. *Int. Conf. Shipp. Chang. Clim.* 12.
- Vianello, C., Carboni, M., Mazzaro, M., Mocellin, P., Pilo, F., Pio, G., Russo, P., Salzano, E., 2020. Hydrogen refueling stations: Prevention and scenario management. large scale experimental investigation of hydrogen jet-fires. *Chem. Eng. Trans.* 82, 247–252. <https://doi.org/10.3303/CET2082042>
- Zanobetti, F., Pio, G., Jafarzadeh, S., Muñoz Ortiz, M., Cozzani, V., 2023a. Decarbonization of maritime transport: Sustainability assessment of alternative power systems. *J. Clean. Prod.* 417. <https://doi.org/10.1016/j.jclepro.2023.137989>
- Zanobetti, F., Pio, G., Jafarzadeh, S., Ortiz, M.M., Cozzani, V., 2023b. Inherent safety of clean fuels for maritime transport. *Process Saf. Environ. Prot.* 174, 1044–1055. <https://doi.org/10.1016/j.psep.2023.05.018>