Modeling Spontaneous Ignition in High-Pressure Hydrogen Jets via Computational Fluid Dynamics and Detailed Reaction Kinetics

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Hydrogen presents unique fire and explosion safety challenges due to its high reactivity, low ignition energy and wide flammability range. In particular, jet fire scenarios involving high-velocity, high-pressure releases of hydrogen have shown spontaneous ignition in the absence of any apparent ignition source such as sparks or flames. Since the early work of Wolanski and Wojcicki (1972), this phenomenon has been observed in various experimental configurations, and several mechanisms have been postulated, including diffusion ignition, reverse Joule-Thomson effects, sudden adiabatic compression, electrostatic and hot surface ignition. Among these, the diffusion ignition mechanism remains the most widely supported, though it requires further investigation in real-scale scenarios.

Experimental investigations have identified spontaneous ignition at relief pressures as low as 2 MPa, but results depend heavily on initial conditions, geometry, and ambient environment. This variability limits the ability to generalize ignition thresholds and to prevent a clear understanding of the mechanisms involved. Experimental approaches alone are not sufficient to resolve the evolution of flow structures and chemical species involved in the early stages of ignition.

Recent computational studies have highlighted the dominant role of shock-jet interactions and vortex formation in promoting spontaneous ignition. The influence of geometrical parameters such as tube length, diameter, and obstacles has been shown to significantly affect both the ignition onset and the subsequent flame structure [1]. Literature CFD models, remain limited by simplified chemical schemes and turbulence-chemistry interaction modeling. In both LES and URANS approaches, sub-grid scale models capable of capturing flame-vortex interactions, coupling with detailed kinetic mechanism and ignition delay under varying conditions are needed.

This research aims to investigate the spontaneous ignition of high-pressure hydrogen jets by coupling fluid dynamics with detailed chemical kinetics. A hierarchy of models with increasing fidelity will be developed and validated against recent experimental data to capture key phenomena such as radical generation, mixing layer growth, and turbulence and vortex effects. Particular attention will be given to transitional behavior between ignition and flame extinction, which is poorly characterized. The final objective is to enhance the predictive capability of CFD models for hydrogen safety assessments and to support the design of mitigation strategies in storage, distribution, and transport infrastructure.

Keywords: *Hydrogen, Spontaneous Ignition, CFD models, Chemical kinetics mechanisms*

Reference

[1] H. Qiu *et al.*, "A review on spontaneous ignition mechanism of pressurized hydrogen released through tubes," *Int. J. Hydrogen Energy*, vol. 86, pp. 613–637, Oct. 2024, doi: 10.1016/j.ijhydene.2024.08.442.