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*CFD based simulation of spontaneous ignition of pressurized hydrogen release*

Computational Fluid Dynamics is an effective tool to investigate and study hydrogen release into air as it has proven to be accurate and less expensive than experimental investigations. CFD can be used to simulate the near exit jet behavior, the dispersion as well as the ignition of hydrogen when release from a compressed hydrogen reservoirs. This presentation will describe a three-dimensional in-house code that was specifically developed to numerically simulate the release from reservoirs with pressures as high as 70 MPa. The sudden release of a pressurized gas into the ambient atmosphere through a small orifice leads to a strong shock wave that is driven by a rapid expansion of the forming jet. In the near exit jet region the flow has an inviscid behavior; therefore the Euler equations can accurately capture this behavior. Since high pressure hydrogen flow deviates from ideal gas assumption, two real gas equation of state are implemented and discussed. Furthermore, a transport equation is needed for calculating hydrogen-air mixture concentration. Simulations are analyzed for different circular and elliptical shapes of the release orifice as well as circular orifices that expand in time. The possibility of spontaneous ignition for different scenarios including different reservoir pressures and different release area shapes is presented based on a simple one dimensional model that examines the conditions at the contact surface between hydrogen and air.