

Predicting Hydrogen Leak Characteristics and Hazardous Behaviour Through Computational Fluid Dynamics and Machine Learning

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The safe management of hydrogen leaks is critical to the growing hydrogen economy, given its easy to leakage, wide flammability range and low ignition energy. This research integrates Computational Fluid Dynamics (CFD) and Machine Learning (ML) techniques to model and predict critical features of unintended hydrogen leaks, such as temperature and concentration profiles, flammability limits, and ignition probability.

Numerical simulations are employed to generate detailed physical data on hydrogen's turbulent diffusion, buoyant rise, and dispersion under various leak scenarios, considering various storage conditions (pressure and temperature). Using the CFD-generated data, ML models such as Random Forest and Gradient Boosting are trained to predict key leak parameters, including temperature gradients, hydrogen concentration distributions, and flammability zones.

Neural networks, specifically convolutional neural networks (CNNs), are applied to capture spatial patterns in the leak dispersion and predict critical thresholds like flammability limits. For predicting the likelihood of ignition, probabilistic models, such as Bayesian networks, are used to integrate factors like hydrogen concentration, temperature, and environmental variables. These ML models enable efficient, real-time prediction of hazardous conditions while significantly reducing the computational overhead associated with CFD simulations. This combined CFD-ML approach offers a powerful tool for improving safety assessments and mitigation strategies in hydrogen storage, distribution, and application systems.

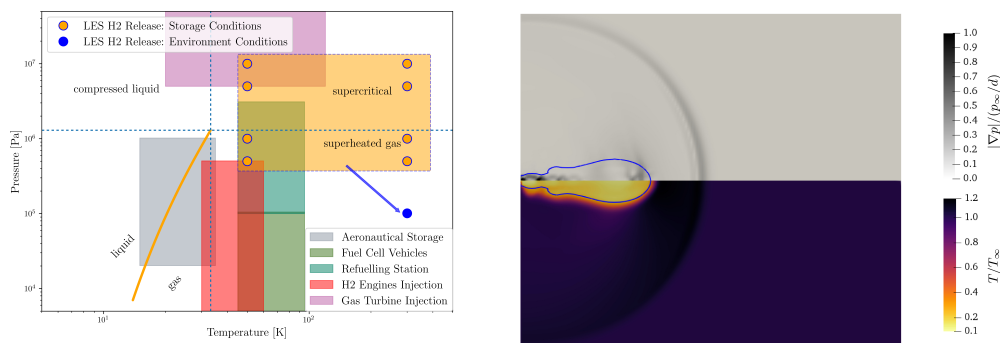


Figure 1: *Left*: Different cases investigated. *Right*: Flow field structure of hydrogen leak from 5 bar and 30 K storage.