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Benchmark Analysis of Accident Modelling Software Applied to Hydrogen Storage

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Global greenhouse gas emissions are reaching unprecedented levels, driving a strong interest in decarbonization. Hydrogen, with applications in industry, transport, and power sectors, offers a CO2- free energy vector when produced renewably. However, the transition to hydrogen as a replacement for fossil fuels presents significant technical challenges including sustainable production and, crucially, safe operation, transportation and storage.

Quantitative Risk Analysis (QRA) encompasses a comprehensive methodology to characterize risks widely used in risk management. Since risk depends on the probability and consequences of failure, accurately estimating consequences is essential for precise risk assessment. Various software tools assist in consequence analysis, and comparing those helps identify their strengths and limitations, improving risk management decisions. In this paper we present a benchmark analysis aimed at evaluating the capabilities of Phast and HyRAM+ software tools in modelling dispersion and fire incidents of gaseous hydrogen from losses of containment in pressurized tanks.

Real-world experimental results have been used as a ground truth for comparing simulation outcomes, ensuring accurate and reliable assessments. Three different experimental studies (Ekoto et al., 2012, Han et al., 2014; Carboni et al., 2022;) were chosen to assess concentration levels of hydrogen clouds, and flame length and radiation exposure from horizontal hydrogen jet fires. Simulated experiments investigated storage pressures ranging from 60 to 400 bar, with release hole diameters spanning from 0.5 mm to 52.5 mm for large-scale hydrogen jets, defined here as flames exceeding 15 meters in length.

A comparison of the results obtained for the dispersion assessment reveals that both software tools generally underestimate hydrogen concentrations, with Phast showing less pronounced underestimation than HyRAM+. On the other side, both software tools generally overpredict flame length, except for slight underpredictions in simulations with the smallest release diameter. For large-scale hydrogen jet fires, Phast tends to overpredict radiation, while HyRAM+ tends to underpredict it. In a QRA framework of hydrogen jets from pressurized tanks, this study suggests that using Phast is preferable due to its more accurate results. However, further validation of the software for large-scale jets is necessary.

* 1. Introduction

Global greenhouse gases emissions are reaching record levels, driving increasing interest in achieving decarbonization. Renewable hydrogen, with applications in industry, transport, and power sectors is climate-neutral and emissions-free, making it a promising solution for sustainable energy (European Commission, 2020). However, hydrogen's safety, particularly in its production, storage, and usage, poses significant challenges. As an extremely flammable gas, hydrogen presents a high risk of fire and explosion accidents due to its wide flammability range (4-75% in air), low minimum ignition energy (0.017mJ), and high heat of combustion (141.6 MJ/kg). It can be easily ignited by sources such as sparks, electrostatic discharges, or mechanical impacts, and fires can escalate in more severe scenarios, especially in industrial settings (Cermelli et al., 2018).

To address these risks, Quantitative Risk Assessment (QRA) is essential. With QRA, the overall risk of hydrogen systems can be systematically quantified, by evaluating both the frequency and consequences of failures leading to loss of containment. Therefore, consequence analysis plays a key role, assessing the potential impact of these accidents on human health and the environment. Various software tools are available for conducting consequence analysis, each employing different models, assumptions and default parameters, which can potentially result in significantly varied outcomes.

In this paper, we present a benchmark analysis using two software tools, Phast and HyRAM+, widely used for consequence assessment. We applied them to evaluate unignited and ignited leaks in pressurized gaseous hydrogen storage systems.

* 1. Methodology

A benchmark analysis is a method used to compare companies, processes, or products within the same sector by using specific indicators (Bhutta and Huq, 1999). In the context of consequence modelling software, it enables the identification of strengths and weaknesses of the tools, guiding the selection of the most suitable one based on the specific goals, accident characteristics, and available resources.

This benchmark analysis compares two consequence modelling software tools: Phast v9.0 (Process Hazard Analysis Software Tool), a proprietary tool developed by DNV for modelling various loss-of-containment scenarios (discharge, dispersion, fires, explosions, and toxic effects), and HyRAM+ v5.1.1 (Hydrogen Plus Other Alternative Fuels Risk Assessment Model), an open-source software developed by Sandia National Laboratories for assessing the safety of hydrogen and other alternative fuels. Experimental studies provided detailed information on initial conditions (release magnitude, temperature, pressure, nature of release) and effects (concentration over distance for the dispersion scenarios and thermal radiation and flame length for the jet fire scenarios). Simulations were conducted with both tools for selected scenarios, and results were compared to experimental measurements to evaluate prediction accuracy.

* 1. Case studies

The experimental studies simulated were chosen based on the completeness of data related to the experimental setup and conditions, ensuring a thorough understanding of the experimental context. Additionally, the clarity and accessibility of the results were considered, to guarantee that the data could be easily compared with the outputs generated by the software tools. Three studies were chosen from the literature to evaluate software accuracy in modelling hydrogen dispersion (Han et al., 2014), flame length (Carboni et al., 2022), and jet fire radiation (Ekoto et al., 2012).

* + 1. Hydrogen dispersion

The capability of the software tools in predicting hydrogen dispersion was evaluated simulating the experimental tests described in Han et al. (2014). In this experimental work, gaseous hydrogen stored in pressurized tanks with a pressure from 100 bar to 400 bar was released horizontally through a hole having a diameter of 0.5 mm, 0.7 mm or 1 mm, resulting in a total of eleven experiments. In each experiment, hydrogen concentration was measured along the jet centreline using five gas samplers placed at distances of 1 m, 3 m, 5 m, 7 m, and 9 m from the jet release point. The typical sampling time was 12 s after the beginning of the release.

Due to the lack of data on wind speed and release height, six simulation sets were conducted with Phast, varying these parameters as shown in Table 1. Atmospheric stability class F and a temperature of 10ºC were assumed based on Han et al. (2014), reflecting calm, clear nighttime conditions. In contrast, HyRAM+ uses a one-dimensional model with Gaussian profiles, accounting for buoyancy but not wind or atmospheric stability, so only one simulation per experiment was performed using its default settings.

Table 1: Wind speed and release elevation conditions tested in jet dispersion simulations carried out in Phast.

|  |  |  |  |
| --- | --- | --- | --- |
| Simulation set ID | Wind velocity (m/s) | Release height (m) | Number of simulations performed |
| S1 | 1 | 0.5 | 11 |
| S2 | 1 | 1 | 11 |
| S3 | 1 | 1.5 | 11 |
| S4 | 1 | 2 | 11 |
| S5 | 0.1 | 1 | 11 |
| S6 | 2 | 1 | 11 |

* + 1. Hydrogen jet fire flame length

To evaluate the ability of the software tools to predict jet fire characteristics resulting from pressurized hydrogen releases, two experimental studies were simulated. The first study, by Carboni et al. (2022), provided data for assessing the accuracy of simulating jet fire flame length. The second study, by Ekoto et al. (2012), was used to evaluate the software's capability to predict radiation from the jet fire at different positions.

Carboni et al. (2022) investigated jet fires from horizontal hydrogen releases at pressures between 90 bar and 450 bar through holes with a diameter of 1 mm, 3 mm, 5 mm, for a total of 17 experiments. Wind speed and direction were recorded at a height of 3 meters by an onsite weather station, with the wind direction aligning with the jet throughout the tests (Carboni et al., 2022).

In the simulations an ambient temperature of 20ºC was assumed, and in Phast, various atmospheric stability classes, based on the Pasquill classification, were tested to determine if this parameter affected the results. Table 2 outlines the atmospheric stability classes tested for each wind speed. In contrast, HyRAM+ requires only the storage and ambient pressure, temperature, discharge coefficient, and orifice diameter as input parameters. Wind effects and atmospheric stability are not incorporated into the software, meaning these factors do not influence the calculated flame length.

Table 2: Atmospheric stability classes investigated in Phast depending on the wind speed.

|  |  |  |  |
| --- | --- | --- | --- |
| Wind velocity (m/s) | Atmospheric stability classes | Number experiments | Number of simulations performed |
| 0 | A, A/B, B, D | 6 | 24 |
| 1 | A, A/B, B, D | 3 | 12 |
| 1.5 | A, A/B, B, D | 1 | 4 |
| 2 | A/B, B, C, D | 7 | 28 |

* + 1. Hydrogen jet fire radiation

The experimental study reported in Ekoto et al. (2012) was used to evaluate the radiation emitted from jet fires at specific points on the experimental site. Compressed hydrogen at around 60 barg was released horizontally through nozzles with diameters of 20.9 mm and 52.5 mm, from a point located 3.25 m above the ground. Wind speed, direction, ambient temperature, and relative humidity were measured about 100 meters upstream from the release point (Ekoto et al., 2012), eliminating the need for assumptions about atmospheric conditions. Radiation was measured using 13 radiometers placed at different locations on the experimental site, with an accuracy of 5% (Ekoto et al., 2012).

* 1. Results

For each case study, the comparison between experimental values and simulation results is shown in Figures 1, 2a, and 2b, with the x-axis representing experimental data and the y-axis the simulation results. Additionally, four statistical metrics were calculated: fractional mean bias (FB), geometric mean bias (MG), normalized mean square error (NMSE), and geometric variance (VG), as defined in Mazzola et al. (2021). An ideal model, with experimental and predicted values always identical, would yield FB = NMSE = 0 and MG = VG = 1.

* + 1. Hydrogen dispersion

As outlined in Table 1, several conditions were tested in Phast. The following considerations can be highlighted (detailed results not shown):

* When varying the release elevation from 0.5 m to 2 m (S1 to S4) and maintaining the wind speed at 1 m/s, the results indicated that as the release elevation increased, the simulated concentration along the jet centreline increased;
* When varying wind speeds (S2, S5, and S6) while keeping the release height at 1 m, the concentration along the jet centreline increased with higher wind speeds near the release point, but decreased at greater distances from the release point. For a wind speed of 1 m/s, the results fell between those calculated for wind speeds of 0.1 m/s and 2 m/s.

Based on the analysis of the different simulation sets, a single value was ultimately selected to compare with the experimental results in Figure 1. This value represents the mathematical average of the results obtained from the simulation sets where the release height was varied, while the wind speed was fixed at 1 m/s. The results from HyRAM+, instead, were directly compared to the experimental values.

The concentrations measured in the experimental study were generally quite low, the majority of data points below the lower flammability limit of hydrogen (4% vol.). As expected, both software tools predicted higher concentrations as the release pressure and hole diameter increased, aligning with the experimental observations. When comparing simulation results with experimental values (Figure 1), most cases showed underestimation, though Phast’s underestimation was less pronounced than HyRAM+. The performance metrics in Table 3 suggest that both tools are comparable: Phast performs better in terms of FB and NMSE, while HyRAM shows better performance in MG and VG.

*Table 3: Statistical performance metrics for Phast and HyRAM+ in dispersion modelling.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Software | FB | MG | NMSE | VG |
| Phast v9.0 | 0.13 | 1.13 | 0.08 | 1.06 |
| HyRAM+ v5.1.1 | 0.16 | 1.04 | 0.11 | 1.05 |



*Figure 1: Hydrogen dispersion. Comparison between experimental results and simulation results. Solid line represents perfect agreement.*

* + 1. Hydrogen jet fire flame length

The simulations conducted in Phast indicated that atmospheric stability class do not significantly influence the characteristics of jet fires. However, this parameter does influence the dispersion of released hydrogen, with increased atmospheric stability leading to higher concentrations of hydrogen downwind.

The comparison of flame lengths predicted by Phast and HyRAM+ against experimental data from Carboni et al. (2022), showed in Figure 2a, revealed that, generally, both software tools tend to overpredict the flame length, with an overprediction exceeding 50% when using a 5 mm release hole diameter (the largest). However, a slight underprediction was observed for the simulated experiments with a release hole of 1 mm. The consistent overprediction is further confirmed by the negative FB value in Table 4. Based solely on the statistical performance metrics, HyRAM+ appears to perform better, which is also evident from the graph, as its predicted flame lengths are closer to the experimental values despite the overall overprediction.

Both Phast and HyRAM+ provide accurate predictions of theoretical behavior by utilizing well-validated correlations to calculate flame length. In HyRAM+, the correlation developed by Houf and Schefer (2007) is specifically used to predict the length of hydrogen jet flames. This model has undergone extensive validation exercises (Ehrhart et al., 2021), demonstrating consistent accuracy in predicting flame lengths for hydrogen jet fires. Similarly, Phast employs the Miller model, which has also been extensively validated, drawing on experimental data from both pilot and full-scale tests (Miller, 2017).

Carboni et al. (2022) used infrared imaging to determine flame lengths, basing the measure on temperature contours. Therefore, the discrepancy between the experimental method and the software definitions of flame length might contribute to the differences observed between simulated and measured flame lengths.

*Table 4: Statistical performance metrics for Phast and HyRAM+ in jet fire flame length modelling.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Software | FB | MG | NMSE | VG |
| Phast v9.0 | -0.33 | 0.75 | 0.17 | 1.14 |
| HyRAM+ v5.1.1 | -0.25 | 0.82 | 0.13 | 1.10 |

* + 1. Hydrogen jet fire radiation

Both software tools allowed to calculate the radiation at specific points defined by their coordinates, simulating the positioning of the radiometers used in the experimental case studies. In the graph showing the comparison between simulation results and experimental values (Figure 2b), each point is complemented with error bars indicating the ±5% accuracy of the radiometers acknowledged in the experimental study by Ekoto et al. (2012).

For the jet fire resulting from a release through a 20.9 mm diameter hole (test 1), Phast consistently overpredicts radiation levels, while HyRAM+ tends to slightly underpredict them. However, for the jet fire from a release through a 52.5 mm diameter hole (test 2), both software tools in most of the cases underpredicted the radiation values at the radiometer positions. Evaluating the overall performance in Table 5, Phast appears to perform better than HyRAM+. Even in cases of radiation underprediction, Phast provides values that are closer to the experimental data.

One possible reason for the underprediction could be the configuration of the experimental setup. It is likely that some of the radiation emitted by the jet fire in test 2 was reflected off the steel sheeting placed on the ground, resulting in increased radiation detected by the radiometers. Since the two software tools cannot account for the reflectance of the material constituting the ground, this additional increase in radiation was not calculated.

*Table 5: Statistical performance metrics for Phast and HyRAM+ in jet fire flame radiation modelling.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Software | FB | MG | NMSE | VG |
| Phast v9.0 | 0.06 | 0.99 | 0.05 | 1.05 |
| HyRAM+ v5.1.1 | 0.32 | 1.40 | 0.26 | 1.18 |

Gráfico, Gráfico de dispersión

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*Figure 2: Jet fire flame length (a) and radiation (b). Comparison between experimental results and simulation results. Solid line represents perfect agreement.*

* 1. Conclusions

A benchmark analysis was conducted to compare the Phast and HyRAM+ software tools, evaluating their accuracy in predicting dispersion, jet fire flame length, and radiation from hydrogen releases from pressurized tanks.

Phast proved to be capable of accurately simulating the experimental setup, incorporating factors like wind velocity and atmospheric stability. However, it slightly underpredicted the experimental values when simulating hydrogen dispersion. It is likely due to assumptions regarding weather conditions and data extraction from the experimental study. When simulating jet fires, Phast generally overestimated flame lengths and showed mixed results for radiation —overpredicting it in one test and underpredicting it in another. This discrepancy may stem from the software's inability to account for ground material reflectance, which can significantly impact radiation levels.

HyRAM+, on the other hand, is a more simplified tool, as it does not account for wind effects, atmospheric stability, or release elevation. The dispersion results generally indicated an underprediction of concentrations. For jet fire characterization, although HyRAM+ also overestimated flame lengths, the overestimation was less significant compared to Phast. However, HyRAM+ consistently underpredicted radiation levels, further emphasizing the need for improved modelling of radiative heat transfer.

To enhance prediction accuracy, particularly in the case of large jet fires, future versions of both software could benefit from incorporating ground reflection effects and employing more comprehensive environmental modeling techniques. This would allow for a more accurate representation of the complex interactions between fire, environment, and radiation, ultimately improving the reliability of the models.

From a practical risk management perspective, these differences in predictions can influence safety assessments and mitigation strategies for hydrogen storage facilities. Overprediction of flame lengths could lead to overly conservative exclusion zones, while underprediction of dispersion and radiation levels might result in underestimated hazard areas. Therefore, understanding the strengths and limitations of each tool is crucial for making informed safety decisions.

In conclusion, considering the features and accuracy of the two tools, Phast is recommended for analyzing hydrogen jet dispersions and jet fires. However, further validation with larger-scale experiments is necessary to enhance confidence in its predictions. Future experimental campaigns should include well-characterized boundary conditions, measurements of ground reflectance effects on radiation, and tests under varying atmospheric conditions to better evaluate software performance under real-world scenarios.

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