NATIONAL LABORATORY OF THE ROCKIES

Development of a Digital Twin for Hydrogen Dispersion and Safety Assessment in an Electrolyzer-Based Hydrogen Production Facility

Preprint

Munjal P. Shah,[1] David Peaslee,[1] Shadi Salahshoor,[2] Rabia Ali,[2] Kevin Hartmann,[1] Jeffery Gifford,[1] Zhiwen Ma,[1] and William Buttner[1]

1 National Laboratory of the Rockies

2 GTI Energy

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DEVELOPMENT OF A DIGITAL TWIN FOR HYDROGEN DISPERSION AND SAFETY ASSESSMENT IN AN ELECTROLYZER-BASED HYDROGEN PRODUCTION FACILITY

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ABSTRACT

Digital twin models are virtual representations of physical systems that use real-time data to simulate and optimize performance. This study presents the development and initial implementation of a digital twin (DT) for the electrolyzer-based hydrogen production facility at the National Renewable Energy Laboratory (NREL)'s Advanced Research on Integrated Energy Systems (ARIES), focused on enhancing safety and optimizing sensor placement through physics-based simulations and metadata integration. The DT incorporates detailed facility-specific information, including component layout, leak locations, and controlled release parameters, to model hydrogen dispersion under varying environmental conditions. Using steady-state computational fluid dynamics (CFD) simulations informed by real meteorological data, such as wind speed, direction, and vertical wind profiles, the DT enables visualization of hydrogen plume behavior and spatial concentration distributions. Comparative analysis between high and low wind speed scenarios illustrates the significant influence of wind dynamics on plume shape and extent, with horizontal momentum dominating dispersion at higher speeds, while buoyancy effects become more prominent under low wind conditions. These simulations generate a rich dataset embedded within the DT, allowing users to assess potential leak outcomes and identify optimal sensor locations based on concentration thresholds. The model supports scenario-based analysis to guide safety strategies and equipment deployment for open-area hydrogen infrastructure. The digital twin thus serves as a dynamic platform for virtual prototyping, providing predictive insight into hydrogen behavior and enhancing risk-informed decision-making. This initial phase establishes a validated foundation for future integration of transient, uncontrolled leak scenarios and real-time sensor feedback, positioning the DT as a critical tool for safety design, operational planning, and adaptive monitoring in hydrogen systems. Overall, the approach demonstrates the value of combining environmental data with digital simulations to inform safer and more efficient deployment of hydrogen technologies.

1.0 INTRODCUTION

Hydrogen demand in the United States currently exceeds 10 million MT annually; this figure is poised to grow substantially both domestically and globally as a hydrogen becomes a leading energy carrier. As industries and governments worldwide seek reliable energy solutions, hydrogen presents an opportunity to stabilize various sectors, improve energy security, and foster economic growth. The expansion of hydrogen infrastructure, including production plants, distribution networks, and refueling stations, has attracted substantial investments from both the public and private sectors [1]. However, ensuring the safe production, storage, and utilization of hydrogen is paramount for its growth [1]. One of hydrogen's key economic advantages is providing a domestic energy carrier thereby mitigating volatility in energy prices and strengthening national energy security [2]. Additionally, advancements in hydrogen production technologies, such as hydrogen generated through electrolysis powered by electricity can enhance grid stability and reliability.

Despite its advantages, hydrogen poses unique safety challenges due to its high flammability, low ignition energy, and ability to form explosive mixtures with air. As hydrogen utilization and adoption increases, stringent safety measures are required to prevent accidents and ensure safe handling across production, storage, and distribution systems [3–5]. Hydrogen leakage detection and mitigation strategies are critical to minimizing risks associated with unintended releases. Computational fluid dynamics (CFD) simulations have been widely employed to analyze hydrogen dispersion behavior and optimize ventilation systems [6,7]. Additionally, sensor-based hydrogen detection technologies are being refined to achieve higher accuracy and response times, improving real-time hazard identification [8,9]. The consequences of safety failures in hydrogen infrastructure have been demonstrated in past incidents. The 2019 explosion at a hydrogen refueling station in Norway, which led to a multi-million-dollar fine for the involved companies, highlighted the critical need for stringent hydrogen safety standards [10]. Similar safety concerns have driven research into advanced detection and mitigation strategies to prevent catastrophic accidents. Hence, the behavior of hydrogen leaks must be thoroughly studied to optimize sensor placement and enhance safety measures. Studies have shown that hydrogen dispersion is highly dependent on environmental conditions such as wind speed, atmospheric pressure, and the presence of ventilation [11,12]. CFD modeling plays a crucial role in predicting hydrogen plume formation and identifying optimal sensor locations in industrial facilities [12]. Effective sensor placement strategies help in early leak detection and minimize the risk of hazardous hydrogen accumulation [13]. Moreover, novel detection strategies, including fiber optic and ultrasonic leak detection methods, are being integrated into safety systems to improve response times and enhance monitoring capabilities [14,15]

Digital twin technology has emerged as a powerful tool in industrial applications, enabling real-time monitoring, analysis, and optimization of physical systems. Since their introduction as concept, digital twins have been widely adopted in industrial applications. Jiang et al. [16] examined their use in manufacturing, automation, and industrial operations, highlighting their transformative impact on predictive maintenance and process optimization. A systematic review by Juarez et al. [17] further explored the broad applications of digital twins across industries, identifying key challenges such as interoperability, data integration, and scalability. Meanwhile, Mihai et al. [18] conducted a comprehensive survey on the enabling technologies for digital twins, discussing their implementation in various sectors, including risk assessment and decision-making. These studies laid the foundation for the application of digital twins in safety management and gas detection systems. Agnusdei et al. [19,20] performed a bibliometric and systematic review to assess the role of digital twins in safety management, concluding that these systems enhance hazard identification, risk assessment, and emergency response. Liu et al. [21] proposed a framework for an indoor safety management system based on digital twin technology, demonstrating its effectiveness in real-time monitoring and risk mitigation. Gas detection is a vital area where digital twins have shown significant potential. Cai et al. [22] introduced a digital twin-based model for natural gas leakage detection, leveraging real-time data analytics for improved hazard mitigation. Similarly, Liang et al. [23] proposed a data-driven digital twin method for leak detection, emphasizing the use of sensor data and machine learning techniques. Wang et al. [24] further explored gas pipeline leakage identification through digital twins, focusing on advanced modeling techniques to enhance detection accuracy. In the realm of hydrogen gas detection, Chaber et al. [25] demonstrated the use of digital twins in high-energy physics experiments, where precise gas monitoring is essential. Yun et al. [26] extended this work by conducting a comparative simulation study on digital twin technology in the gas industry, underlining its potential for hydrogen safety applications.

While current digital twin applications in safety rely heavily on real-time data analysis, there is a growing interest in integrating predictive modeling capabilities, stand-alone digital twins for system behavior modeling, and digital twins for simulation and modeling purposes. Hence, this study aims to develop a digital twin for safety and sensor placement purposes for National Renewable Energy Laboratory's Advanced Research on Integrated Energy Systems (ARIES) testbed. ARIES has a 1.25-MW electrolyzer for hydrogen production. This facility is also being developed for hydrogen sensor testing in open area to facilitate part-per-million (ppm) to part-per-billion (ppb) level testing and verification. The facility can do controlled hydrogen release rate up to 22 kg/hr. By leveraging this controlled release capability, we can test and evaluate sensors under real word scenarios. Digital twin model for the facility will be useful in deployment of sensors based on their sensitivity and range and identifying potential hazard areas on site for the controlled and uncontrolled releases. We have used computational fluid dynamics (CFD) based simulations to model hydrogen dispersion behaviour on site under open area release scenarios. The study presented here aims to outline current progress, steps for development of digital twin and future steps to incorporate predictive modelling.

2. METHODOLOGY

As mentioned, National Renewable Energy Laboratory (NREL) houses a 1.25-MW proton exchange membrane (PEM) electrolyzer based hydrogen production facility at the Flatirons campus as part of ARIES testbed [11]. The digital twin (DT) implementation for ARIES hydrogen facility involved multistep process as depicted in Figure 1. Currently, the first two steps have been implemented. Metadata of physical twin were modeled into Digital twin. The hydrogen production testbed physical twin and digital twin are shown in Figure 2. The facility has 16 various components mentioned in Figure 2(e). As the goal of digital twin is safety and sensor placement, the digital twin includes relevant metadata on potential controlled release and uncontrolled leak locations of the site.

As part of Step-2, hydrogen dispersion from main process vent stack was modeled., with steady-state data generation and implementation in DT achieved. To generate the dataset, we utilize metadata from facility on leak rate and locations. Two vent stakes are designed to release processed gas into the ambient environment: (1) the vent stack located on gas management panel (marked as 16 in Figure 2(c)) and (2) the main process vent on electrolyzer (marked as 10 in Figure 2(c)) which is visible as the vertical pipe. For initial dataset and implementation, we have used (2) the main process vent on electrolyzer for modeling.

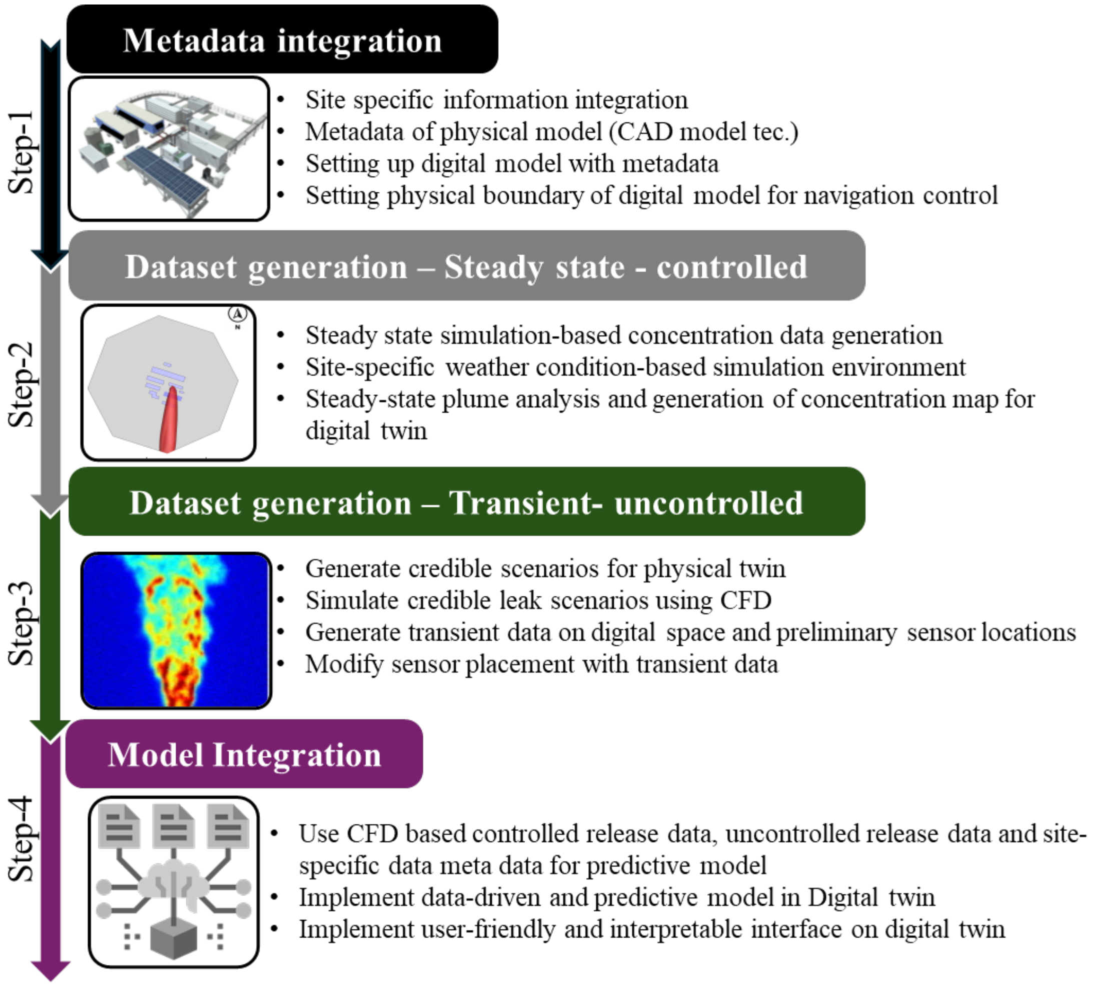


Figure 1. Development steps as part of the digital twin modelling

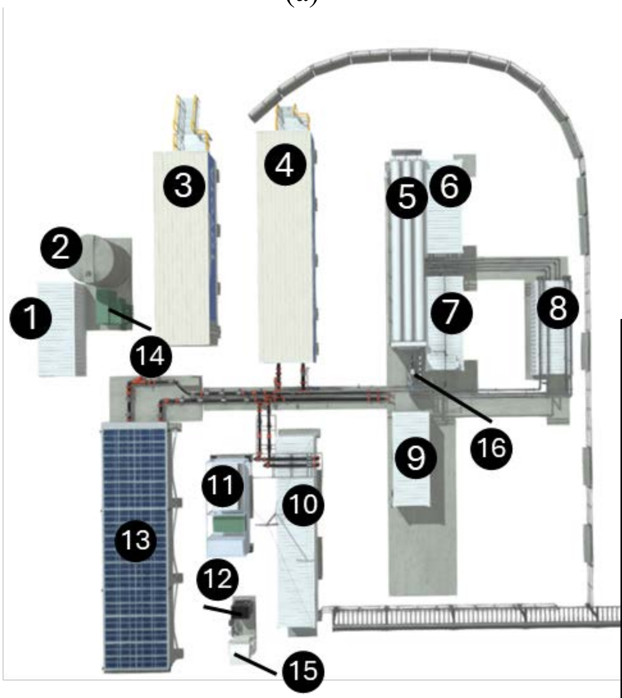
For steady-state data generation, on-site weather data like atmospheric wind profiles (i.e., wind speeds as a function of height) and wind direction were taken into account. Weather data were collected for during the entire FY23 calendar year i.e. 1st Jan 2023, to 31st December 2023 from Measurement and Instrumentation Data Center (MIDC) M2 data collection tower on site [27]. Weather data was extracted for non-precipitation hours and compiled into a dataset. A wind rose plot of the site wind patterns is shown in the Figure 3(a). It is evident that high velocity winds are predominantly coming from W to N region (i.e., 270-360 degrees). ; the structures at the site are aligned with that wind direction.. The scatter plot with histogram sheds light on distributions of windspeeds and direction. Although NW is predominant direction, site experiences winds from all directions as evident by Figure 3(b) (top histogram for angle). Most probable windspeed observed are below <10 m/s as evident from skewed distribution with outliers for high wind speeds.

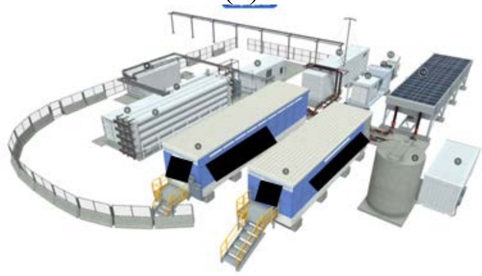
To model wind speed in simulation, we adopted power law exponent-based profile. Wind typically follows a power law relationship with distance from ground. We have measurement points for speed at elevations of 2, 5, 10, 20, and 50 m available on site. Based on the data we can calculate power law exponent, β, from linear regression using,

$$\frac{u}{u_{2m}} = \left(\frac{h}{h_{2m}}\right)^{\beta} \rightarrow \ln\left(\frac{u}{u_{2m}}\right) = \beta \ln\left(\frac{h}{h_{2m}}\right) \rightarrow u^{*} = \beta h^{*} \qquad (1)$$

Where, u is wind speed at given elevation, u_{2m} is wind speed at 2 m elevation from the ground. β is the power law exponent, h_{2m} is 2 m, h is the elevation from the ground. From this equation, we can calculate wind speed at any height using the u at 2 m elevation and β.

(a) (b)





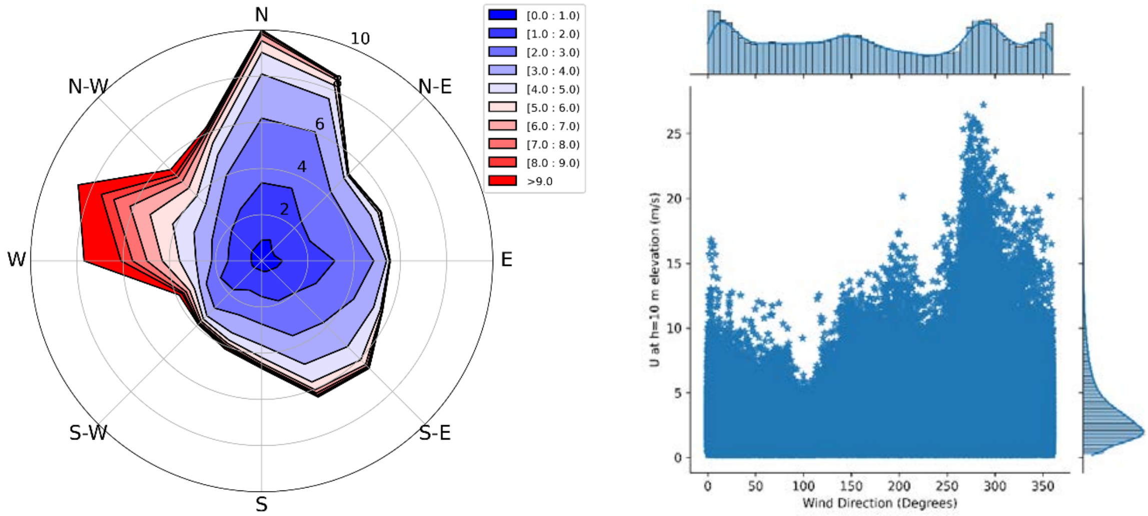
(d)

No	Description
1	DI Polishing System
2	Water Storage Tank
3	1 MW PEM Fuel Cell (electronics enclosure)
4	1 MW PEM Fuel Cell (H2 enclosure)
5	15 LP Tanks (600 kg)
6	GKN Mega Tank
7	GKN Mega Tank
8	Thermal Management System
9	Compressor
10	PEM Electrolyzer (H2 enclosure)
11	PEM Electrolyzer (electronics)
12	Chiller
13	Dry Cooler System
14	Transformer
15	HVAC
16	Low Pressure Gas Management Panel (LP GMP) Con-trols

(c) (e)

Figure 2 (a-b) Hydrogen production facility on ARIES site i.e physical twin (c-d) Digital twin model with the metadata of site included in model (e) list of components for site with information.

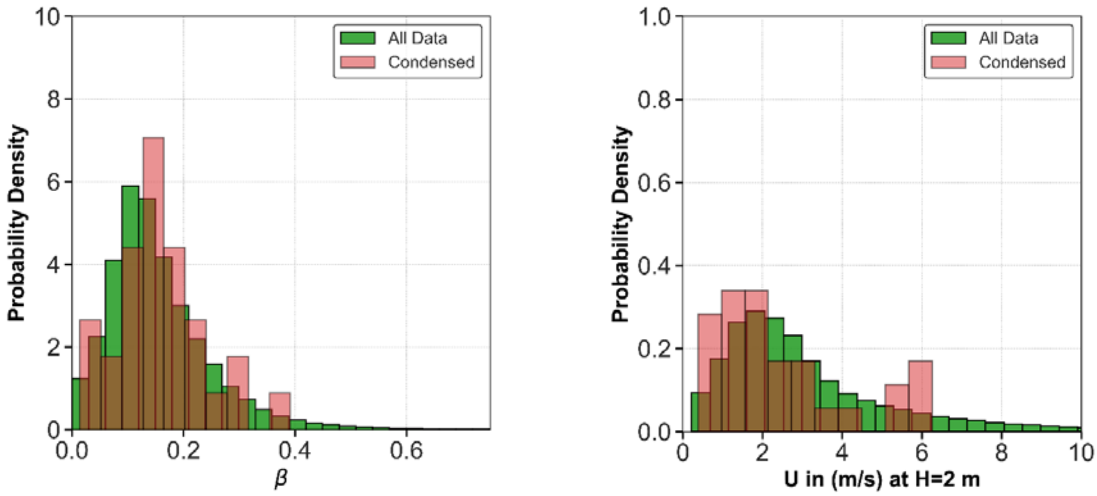
To reduce the weather conditions to model for dispersion, a statistical approach was chosen. For variables of interest i.e. wind speed at 2 m/s and wind profile power-law exponent (β) a Kolmogorov-Smirnov test was conducted to determine if a condensed and a full dataset share same distribution or not. It was determined that the condensed and full datasets shared same distribution with p=0.21 and 0.24 ($p>0.05$) found for u and β sets, respectively.



(a) (b)

Figure 3 (a) Wind rose plot showing the direction and magnitude of wind speed data collected for ARIES site (b) Distribution of wind speed vs wind direction for the site with histogram of each for common experienced weather conditions for FY23 at elevation of 10 m.

In total 30 various windspeed parameters (u_{2m} and β) were selected for simulation input parameter space. The distribution of all data for FY23 and condensed data of 30 conditions are shown in Figure 4. It is evident that condensed data follows the parent data distribution. Using the condensed data for wind speed and 8 directions (N, NE, E, SE, S, SW, W, NW), we formulated scenarios to model for the steady state plume dataset for DT model. Hence, we simulated 30 different wind profiles for 8 different wind directions on ARIES site i.e., 240 scenarios in total.



(a) (b)

Figure 4 All year weather data and condensed for (a) wind profile power-law exponent (β) and (b)wind velocity at 2 m/s.

We implemented an octagon shaped model for simulating ARIES site as wind direction varies a lot for scenarios. A schematic of the model implemented in our simulation framework using ANSYS Fluent is shown in Figure 5. Based on wind direction, 8 sides of domain dynamically switch to inlet and outlet. This way we can account for various wind direction and profiles into modelling. The simulations were done using steady-state assumption to model hydrogen plume. Steady-state assumptions were used because hydrogen dispersion reaches a steady-state distribution (i.e., plume) quickly given fixed wind conditions. The variability in wind condition is complex and was handled by simulating the 240 different conditions, as mentioned.

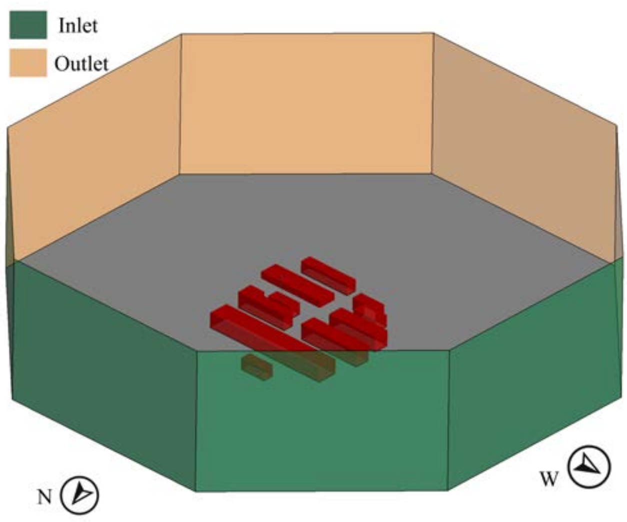


Figure 5 Octagon domain to account for wind direction variations in CFD simulations. Example inlets and outlets marked for a wind coming from north.

We conducted modeling on the computational domain with Reynolds Average Navier-stokes (RANS) with k-w SST turbulence model with full buoyance effects within our computational framework developed in ANSYS Fluent. To solve hydrogen dispersion, we employed species transport modeling approach solving conservation equations describing convection and diffusion of each component species i.e., H_2, N_2, O_2. We also calculated the effect of enthalpy transport due to species diffusion in the energy equation. Again, all simulations conducted were steady state. Computational domain was discretized in ~3 million elements. Second order or higher discretization schemes were used for solving pressure, velocity, energy, and species. It is also to note that ideal gas was used for computations as hydrogen is at ambient conditions. Although our framework is steady state, we have also validated our framework with the work of Giannissi et al.[28] for a flow rate of 18 Liters/minute flow rate in a closed facility for transient conditions.

3. RESULTS AND DISCUSSION

Different weather conditions were incorporated into CFD, and scenarios were modelled. The resulting plume for each scenario changes as wind power law coefficient, speed, and direction changes for each simulation. Figure 6 shows a low (0.6m/s) and high wind speed (7.6 m/s) plume comparison for the same wind direction. It compares the iso-surfaces of hydrogen concentration above 0.05% volume. It is evident from the plume size that with high winds hydrogen dispersion is predominantly due to the momentum of flow and dispersion is mainly horizontal. However, with the low wind conditions, hydrogen buoyancy affects dispersion. Although dispersion direction remains horizontal, plume rises vertically due to buoyancy. In high wind scenarios, horizontal momentum dominates dispersion, and more than buoyancy could affect plume, it disperses quickly. Consequently, we can see that for same volume concentration the high wind speed cloud is smaller than low speed. In the context of hydrogen safety, high wind speeds are very helpful in dispersing hydrogen away from leak location. However, high wind speeds are not commonly observed phenomenon as well. Low wind speed scenarios are also likely to occur which may sway hydrogen cloud vertically but closer to the original leak location. The dataset generated would help in identifying sensors and its locations for open facilities. To support this, a comparison of low and high wind speed with various concentration cloud are shown in Figure 7. It highlights concentration levels >0.01%,>0.1%, and 1% volume. As explained above, at high wind speeds hydrogen disperses quickly and hence cloud size is smaller that of the high wind speed scenarios. High concentration cloud for both scenario is still closer to vent stack and a small region. It is to note that, initial dataset generation was done from vent stack which is 10 m high. Although this is by design, not all facility will have vent stack that high and are likely to have secondary release locations and credible uncontrolled leaks closer to equipment's on site.

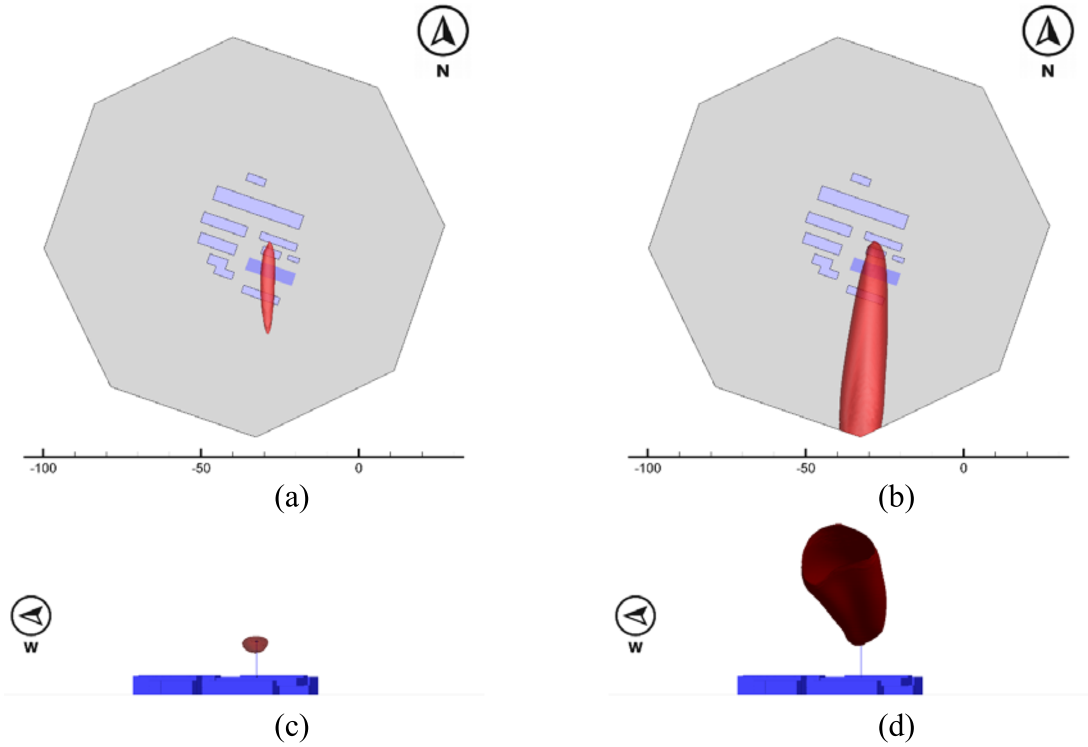


Figure 6 Hydrogen plume cloud (In red) above 500 pm (0.05 vol % or higher) for (a-c) High wind scenario at 7.6 m/s and (b-d) Low wind scenario at 0.6 m/s (a-b) are top eagle eye view for plume and (c-d) are side views from ground. Scale on the bottom is in meters.

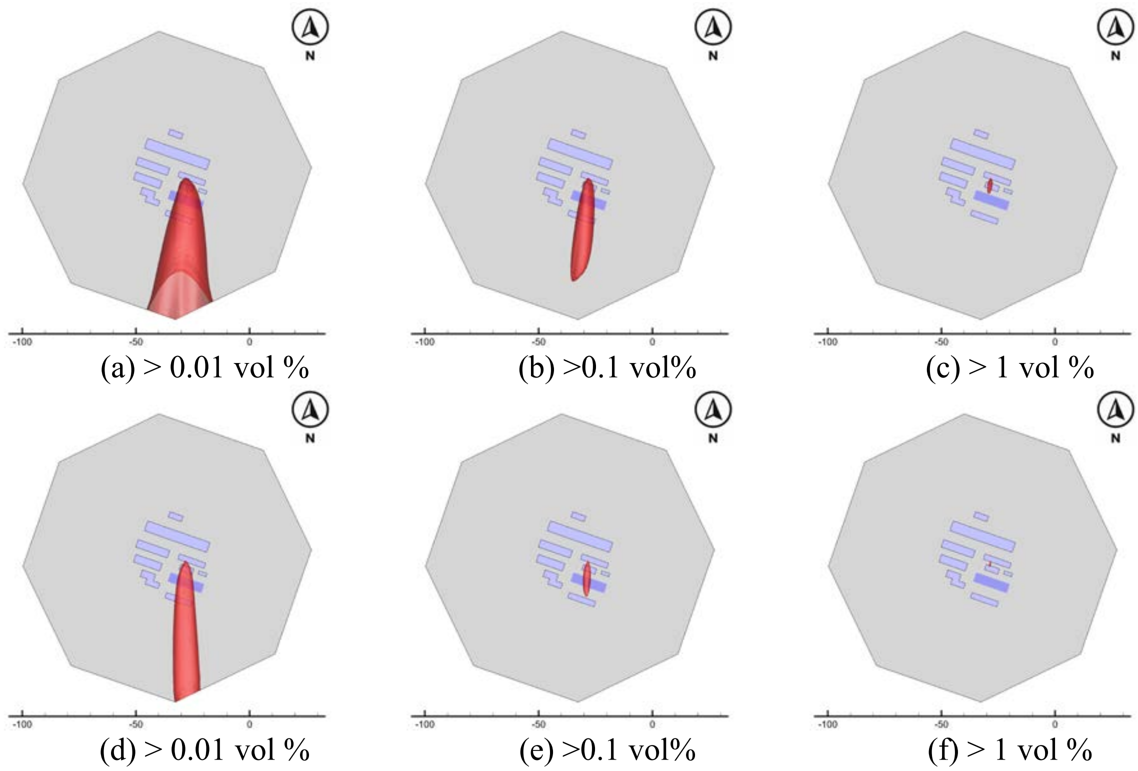


Figure 7 Effect of wind on concentration level of hydrogen near site. Highlighting dispersion behaviour of hydrogen with wind.

It is clear that wind patterns would dominate hydrogen dispersion. For sensor placement of open area hydrogen facilities, digital twins could help visualize potential leak scenarios and hydrogen concentrations across site. They will also help visualize potential regions for sensor placement based on their ranges. For example, for a sensor with the detection range below <100 ppm would be most ideal away from the site, where as a detector with higher detection range say >1% volume would be ideal, closer to components on site.

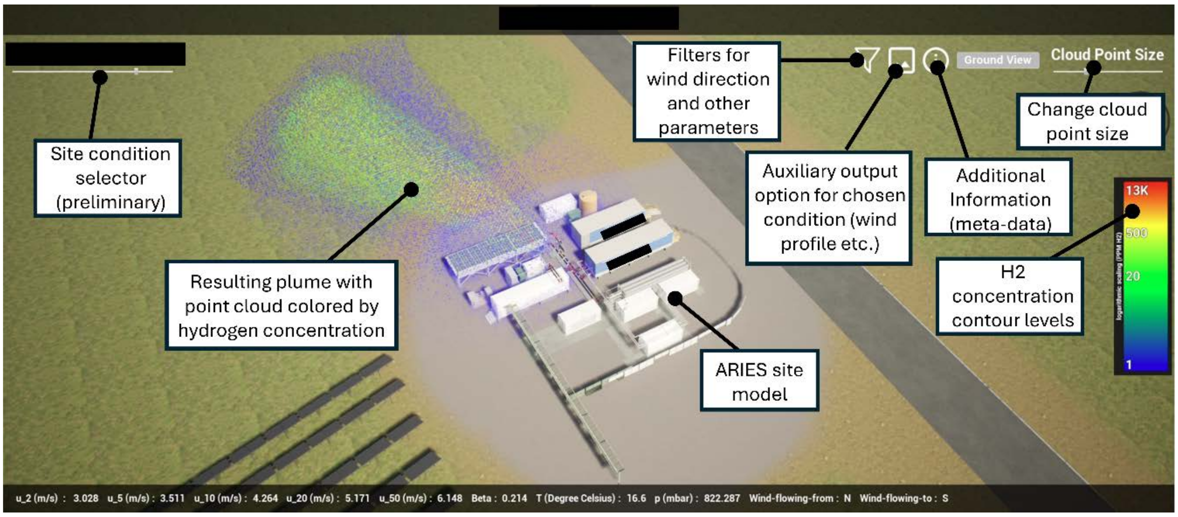
The dispersion analysis presented here is essential to building basic components and attributes of digital twin. A digital twin based on modelling data is presented in the Figure 8. Table 1 summarizes the identified attributes and their use for digital twin purposes. These attributes collectively support the goals of safety evaluation and sensor placement optimization in the hydrogen facility's digital twin, with steady-state simulations currently implemented using real meteorological and facility metadata.

Table 1. Various attributes and description of each in digital twin interface

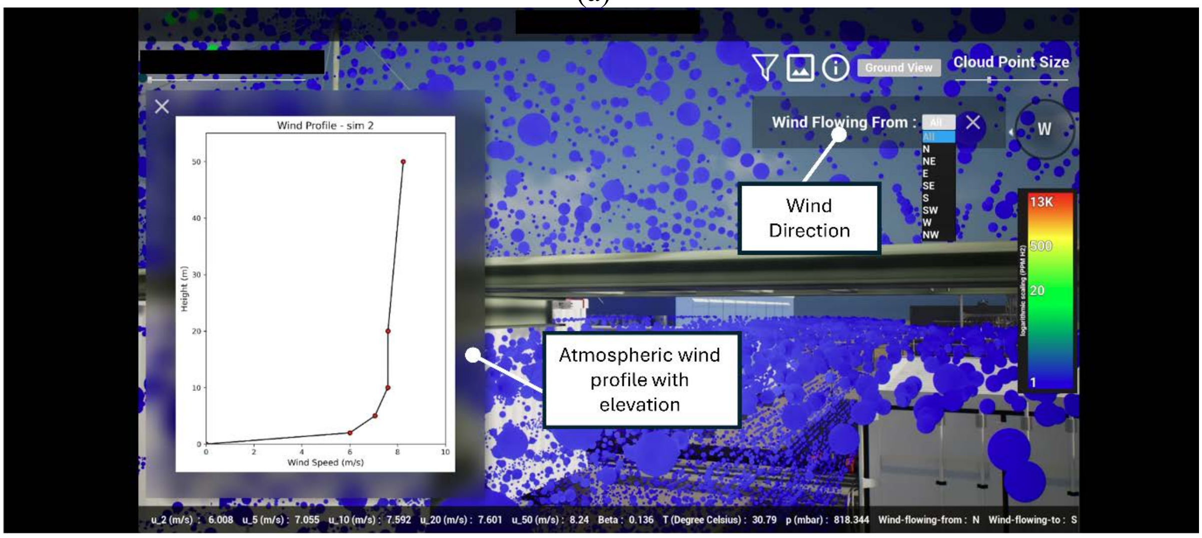
Attribute	**Description / Use in Digital Twin**
ARIES Site Model	3D digital representation of the physical site, including structures, stack positions, etc.
Site Condition Selector (Preliminary)	Allows switching between different predefined scenarios or weather conditions for simulations.
Hydrogen Concentration Point Cloud	Visualizes the plume of hydrogen dispersion; color-coded by concentration for safety assessment.
Wind Filters (Direction, Parameters)	Filters data based on wind direction to study specific scenarios and assess impact from all angles.
Ground View Selector	Changes perspective to ground level to analyze plume behavior and hazard zones from ground level.
Cloud Point Size Selector	Adjusts visualization resolution to highlight dense or sparse gas concentrations.
Auxiliary Output Selector (Wind Profile, etc.)	Shows relevant output such as wind profile data for better environmental context during simulation.
Additional Metadata Information	Displays information like release location, wind speed, stack dimensions for model transparency.
H_2 Concentration Contour Levels	Color scale that defines hydrogen concentration values for hazard analysis and sensor placement.
Wind Direction Indicator	Shows wind flow direction, critical for modeling plume dispersion and guiding sensor positioning.
Atmospheric Wind Profile with Elevation	Plots vertical wind speed distribution; used for setting boundary conditions in CFD simulations.
Steady-State Data Visualization	Represents controlled leak scenarios under constant wind, important for base model validation.
Transient Scenario Integration (Planned)	Upcoming feature to simulate uncontrolled leaks under variable conditions for emergency preparedness.
Model Integration Pipeline (Planned)	Integrating ML/AI or real-time predictive safety analytics.

The hydrogen dispersion simulations under varying wind conditions have substantially contributed to the advancement of the digital twin framework for the ARIES hydrogen facility. By modeling the influence of environmental factors such as wind speed and direction on gas plume evolution, the digital twin now incorporates dynamic representations of potential leak scenarios. The generated data delineates how plume shape, extent, and orientation shift in response to atmospheric variability, offering a detailed spatial understanding of dispersion behavior.

Digital twin provides users with a visual and quantitative tool to explore how hydrogen behaves under differing environmental loads, informing strategic decisions about facility layout, operational planning, and safety design. More specifically, the simulation outcomes will guide the placement and selection of gas detection equipment, aligning sensor deployment strategies with expected concentration levels across various regions of the site. The extension of this work will allow users to select the range of concentrations to show probable map of sensor location of their choice. The digital twin thus evolves from a static model into a responsive, data-driven platform capable of supporting proactive risk mitigation and optimizing hydrogen safety infrastructure.



(a)



(b)

Figure 8 Digital twin interface with each attribute of interface marked with explanation. (a) Eagle eye view of site from digital twin (b) view closer to site components.

4. CONCLUSIONS

The current implementation of the digital twin (DT) for the ARIES hydrogen facility encompasses metadata integration and steady-state hydrogen dispersion modeling. Using facility-specific data such as leak locations, release rates, and atmospheric wind profiles collected over the FY23 calendar year, the DT simulates controlled releases from the main process vent stack. The point cloud visualization of hydrogen concentration, combined with directional wind filtering and elevation-based wind profiles, enables accurate representation of gas dispersion patterns under various site conditions. This foundational phase is significant as it establishes a validated baseline for understanding plume behavior, supports preliminary safety assessments, and informs optimal sensor placement strategies, thereby laying the groundwork for future expansion into more complex and dynamic simulation scenarios.

The future steps outlined for the digital twin of the ARIES hydrogen facility present significant opportunities for advancing safety analysis, risk mitigation, and system optimization through highfidelity modeling and data-driven integration. With the planned inclusion of humidity in the modeling, transient and uncontrolled release scenarios, the DT framework can be extended to simulate complex accident conditions under dynamically changing environmental parameters. This advancement will enable the evaluation of worst-case dispersion patterns and their interactions with site infrastructure, enhancing preparedness and response strategies. Additionally, the integration of sensor data and machine learning models within the DT architecture offers the potential for predictive diagnostics and anomaly detection. Such capabilities could facilitate informed decision-making for operational safety. Furthermore, the continued assimilation of metadata, including structural configurations and leak characteristics, supports the refinement of CFD-based simulations, making the DT a robust tool for virtual prototyping, sensor placement optimization, and training applications. Ultimately, the comprehensive development of this digital twin can serve as a model for hydrogen infrastructure risk management and design validation.

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