NREL

Development of a digital twin for hydrogen dispersion and safety assessment in an electrolyzer based hydrogen production facility

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Photo by Josh Bauer, NREL 61725

Motivation

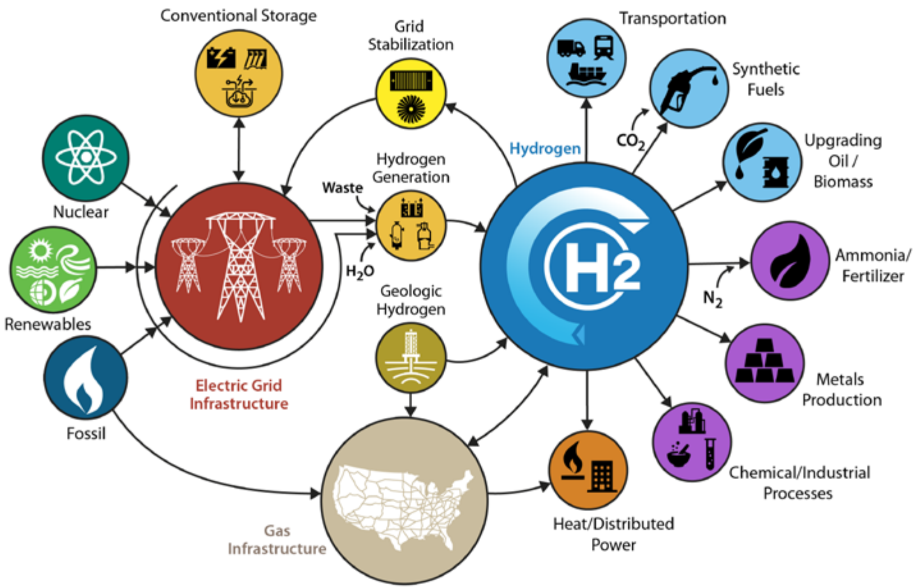
Important safety questions:

- How can facility metadata be integrated into a digital twin for hydrogen safety?
- What steady-state conditions can be modeled to establish controlled baseline scenarios?

Our approach:

- Build Computational fluid dynamics (CFD) models of a hydrogen facility.
- Conduct validation/comparison studies with controlled releases.
- Use CFD model to perform hydrogen dispersion scenario analysis.
- Use model outputs to optimize sensor placement and detection strategies.
- Provide a validation platform for sensor developers through the digital twin.

H2@Scale



Reasons for Detection and Monitoring

- Provide assurances of safety
  - Avoids accumulation and potential for delayed ignition
  - Activate warning alarm and system shutdown
  - Alleviate concerns of community stakeholders
- Minimize product waste (emissions monitoring)
  - Desired monitoring range of interest (ppm_v)
  - Market driven / application specific
- Process control applications (up to 100 vol%)
  - Fuel Composition/Fuel Quality and metrology
- Released hydrogen behavior modeling validation
  - Impacted by environmental and facility parameters
  - Inform sensor deployment strategies
- Prognosis and Health Management (PHM) Applications
  - Improve reliability and cut maintenance cost

The impact of delayed ignition arising from an undetected (and unexpected) hydrogen release and accumulation can be illustrated in *"Hydrogen refueling plant explodes in Norway."* see https://ctif.org/news/hydrogen-refuelling-plant-explodes-norway

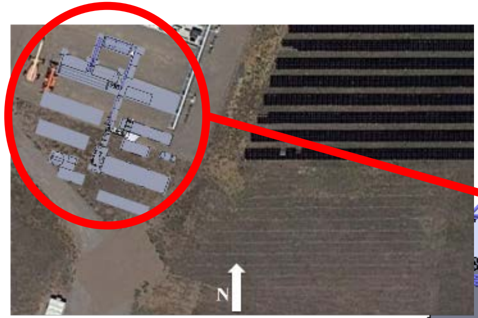
Gas sensors represent the most common strategy for the direct detection of hydrogen releases. Delayed ignition of accumulated released hydrogen MUST be avoided

NREL Flatirons Facility

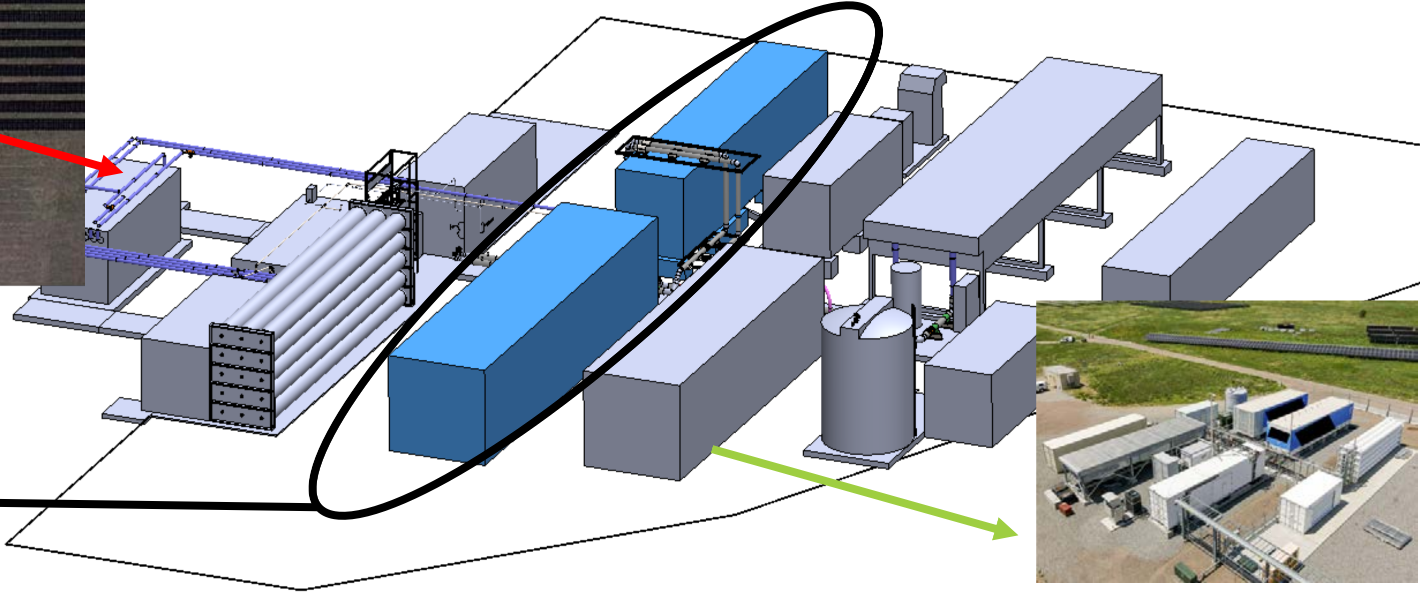
Aerial view of the hydrogen infrastructure and grid integration research pads at National Renewable Energy Laboratory's (NREL's) Flatirons Campus.

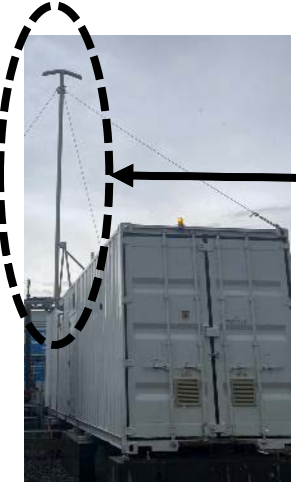
Unique site location of **ARIES (Advanced Research on Integrated Energy Systems)**

Outdoor hydrogen dispersion modeling



ARIES (Advanced Research on Integrated Energy Systems) testbed





Modeling outdoor hydrogen releases at ARIES (Test bed for release studies)

– 22.4-27 kg/hr release rate
– 0.84 bar avg. ambient pressure
– Historically representative wind speed & direction

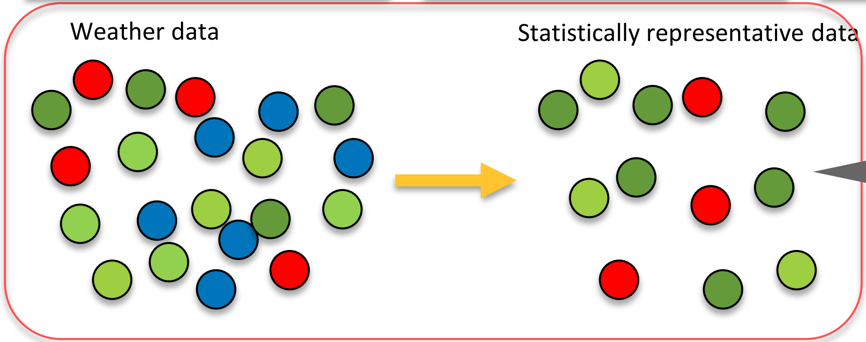
Modeling integrates leak and site parameters (e.g., wind, weather and structures)

- Sensor placement strategies (short-term)
- Emissions profiling and source location (longer-range goals)

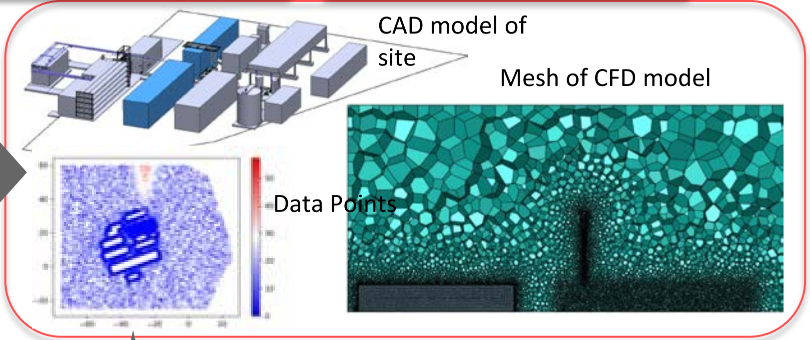
Hydrogen leak Modeling

Developed pipeline for sensor placement strategy

Site specific weather information → Site specific CAD and CFD modeling → Data processing of H_2 concentration → Digital twin integration

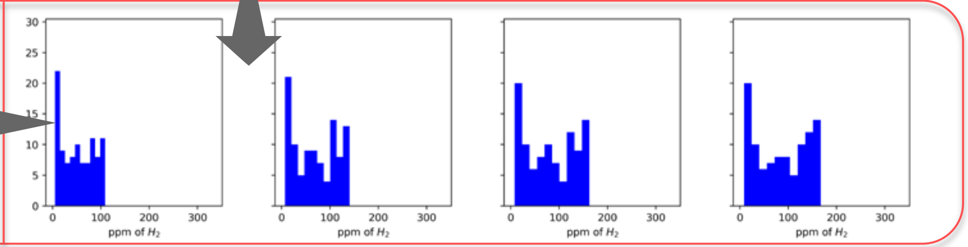


Atmospheric conditions



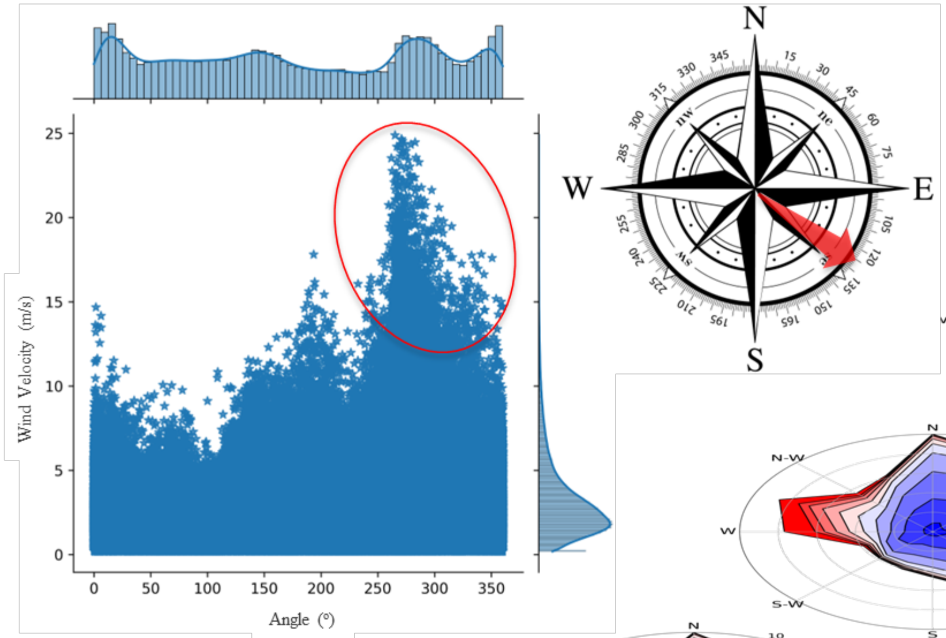
*~ **N** steady state CFD simulations*

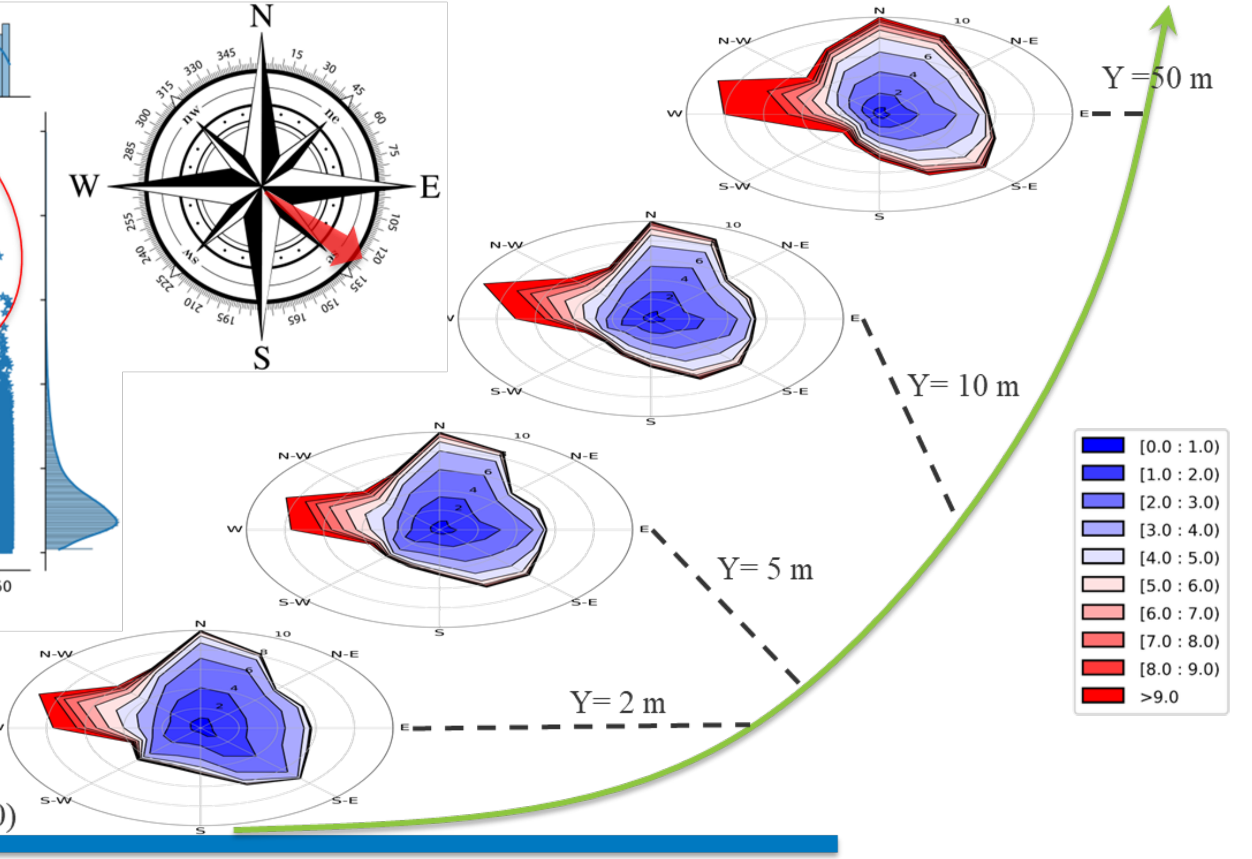
Digital twin Integration



H_2 concentration map at various locations of interests on site

Wind conditions on site

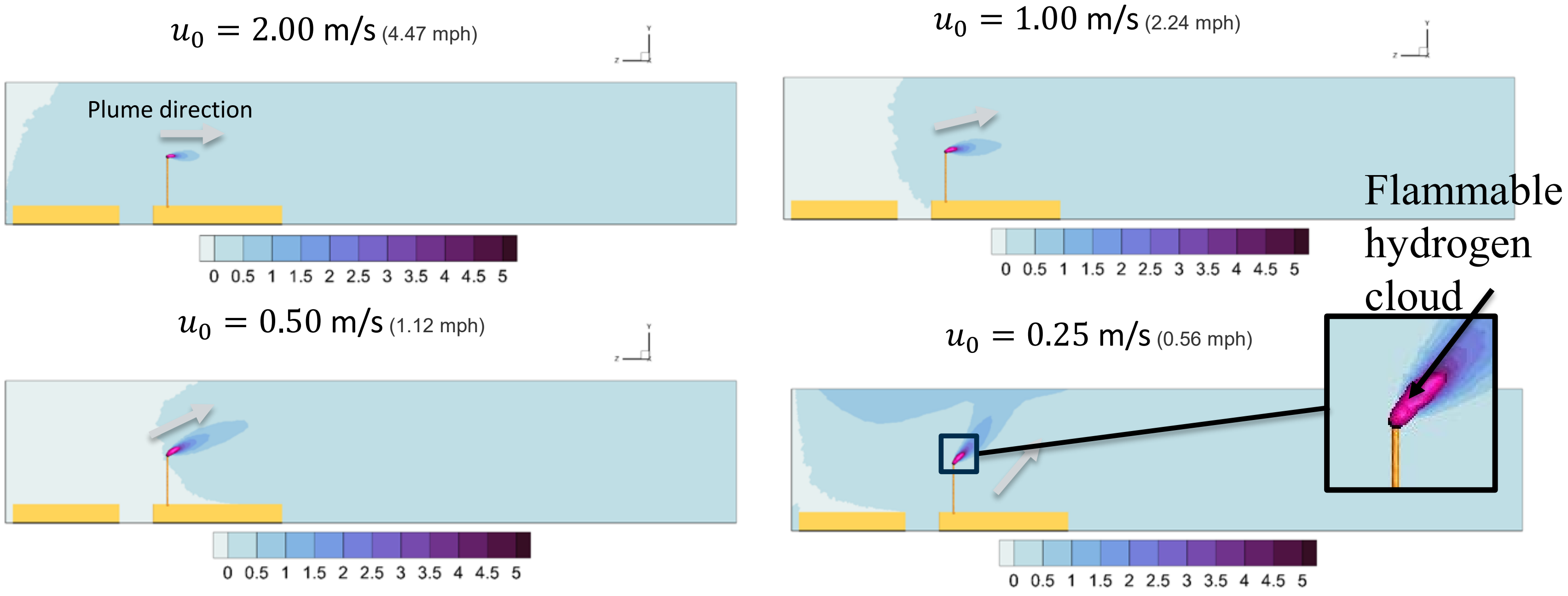




Windrose maps at various elevation for 1 year data (Jan-1 to Dec -31)

H_2 dispersion behavior

Hydrogen dispersion nature is wind dependent

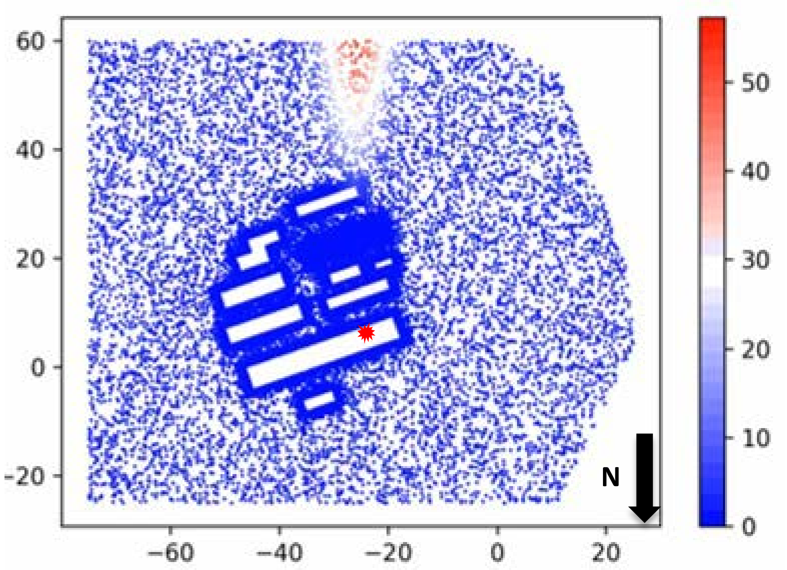


Hydrogen Sensor Measurement Range →

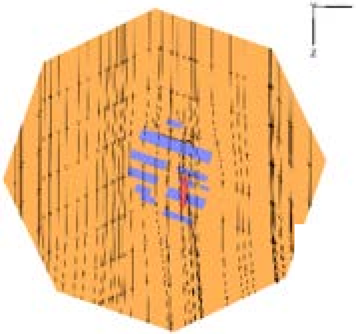
1. Near to leak - **vol% range**
2. Away from leak and around site - **< 500-1000 ppm**
3. Downstream of leak - **<10-100 ppm**

CFD modeling and statistical sampling

- 240 simulations for 1 year weather data (30 unique wind conditions) and 8 wind directions (45º interval)

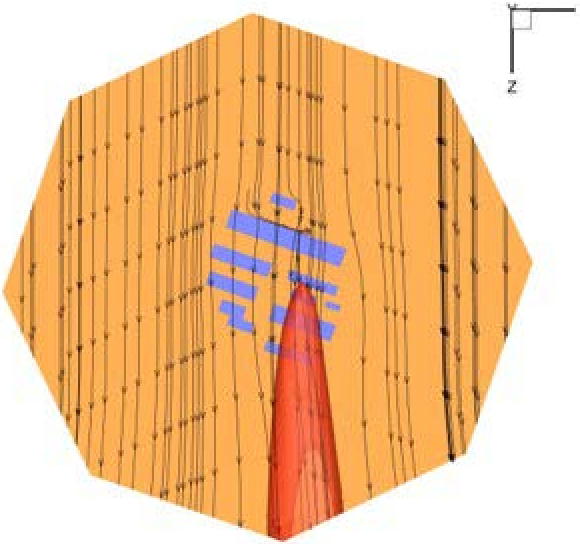


~1 M data point tracked over 240 simulations



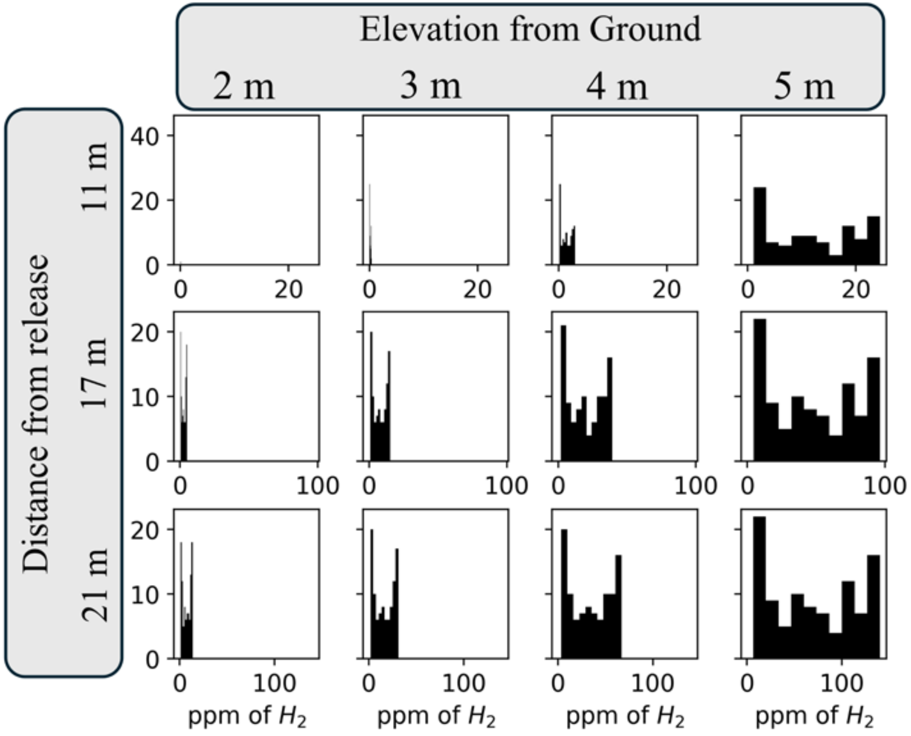
Propagation of hydrogen cloud after leak at 26 mph of wind

H2 leak simulation for ARIES site. Red region highlighting cloud of hydrogen above 20 ppm.

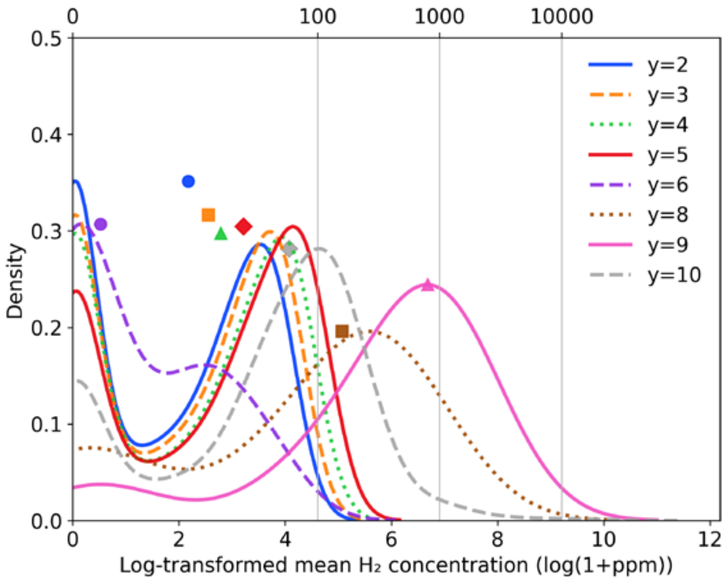


Large data ensemble and processing techniques for simulation-based approach

Analysis of hydrogen dispersion



Statistical quantities of average hydrogen concentration in logarithmic (bottom axis) ppm and raw ppm at various elevations

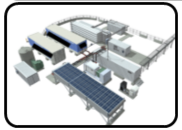


Distribution of hydrogen concentration downstream of the site and at various elevation, showing effect of buoyancy relative to release location

Digital twin

Step-1

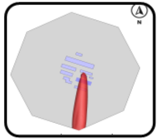
Metadata integration



- Site specific information integration
- Metadata of physical model (CAD model tec.)
- Setting up digital model with metadata
- Setting physical boundary of digital model for navigation control

Step-2

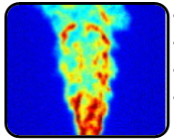
Dataset generation – Steady state - controlled



- Steady state simulation-based concentration data generation
- Site-specific weather condition-based simulation environment
- Steady-state plume analysis and generation of concentration map for digital twin

Step-3

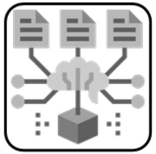
Dataset generation – Transient- uncontrolled



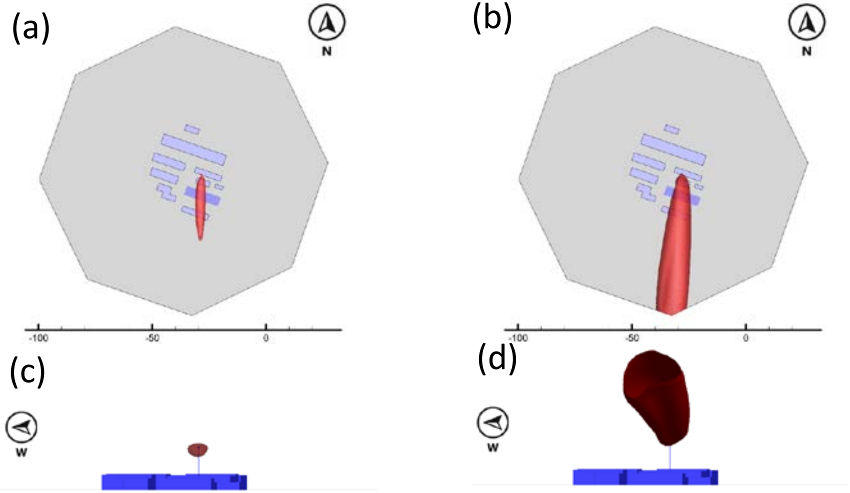
- Generate credible scenarios for physical twin
- Simulate credible leak scenarios using CFD
- Generate transient data on digital space and preliminary sensor locations
- Modify sensor placement with transient data

Step-4

Model Integration

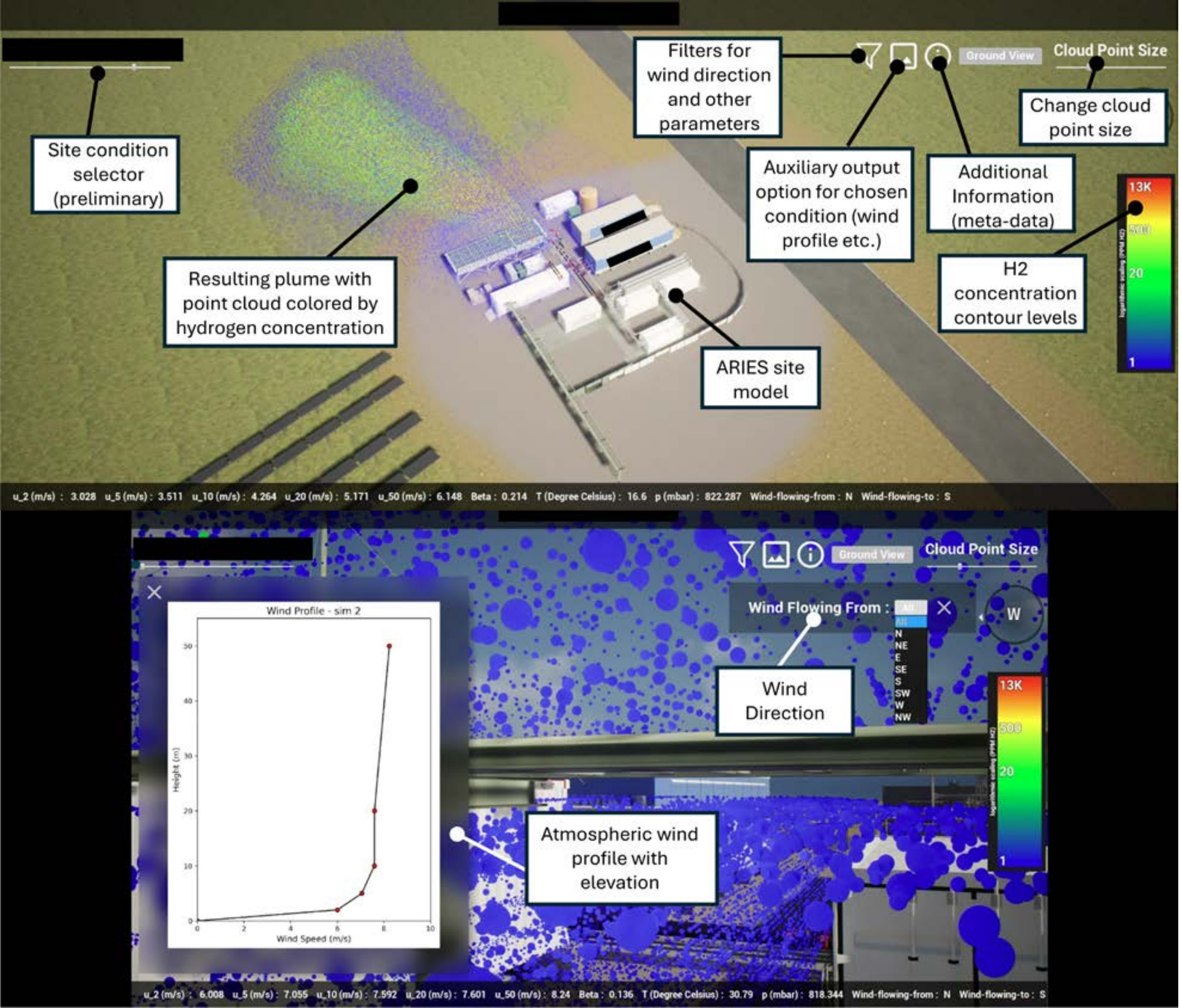


- Use CFD based controlled release data, uncontrolled release data and site-specific data meta data for predictive model
- Implement data-driven and predictive model in Digital twin
- Implement user-friendly and interpretable interface on digital twin

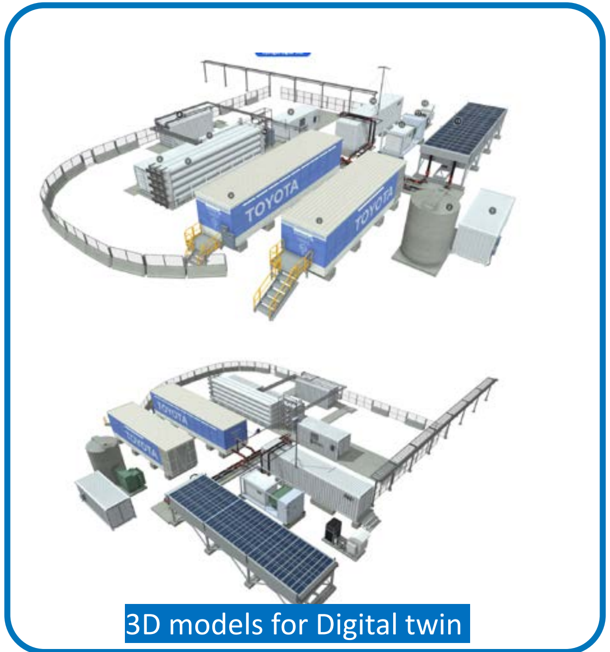


Hydrogen plume cloud (In red) above 500 ppm (0.05 vol % or higher) for same wind direction and leak rate (a& c) **High wind scenario at 7.6 m/s** and (b& d) **Low wind scenario at 0.6 m/s** (a-b) are top eagle eye view for plume and (c-d) are side views from ground. Scale on the bottom is in meters.

Digital twin incorporating the site-specific conditions


[redacted]
[redacted]
Filters for wind direction and other parameters
Ground View
Cloud Point Size
Change cloud point size
Site condition selector (preliminary)
Auxiliary output option for chosen condition (wind profile etc.)
Additional Information (meta-data)
13K
500
20
1
H2 concentration contour levels
Resulting plume with point cloud colored by hydrogen concentration
ARIES site model
u_2 (m/s) : 3.028 u_5 (m/s) : 3.511 u_10 (m/s) : 4.264 u_20 (m/s) : 5.171 u_50 (m/s) : 6.148 Beta : 0.214 T (Degree Celsius) : 16.6 p (mbar) : 822.287 Wind-flowing-from : N Wind-flowing-to : S
[redacted]
Ground View
Cloud Point Size
Wind Profile - sim 2
Height (m)
Wind Speed (m/s)
Wind Flowing From :
All
N
NE
E
SE
S
SW
W
NW
W
Wind Direction
13K
500
20
1
Atmospheric wind profile with elevation
u_2 (m/s) : 6.008 u_5 (m/s) : 7.055 u_10 (m/s) : 7.592 u_20 (m/s) : 7.601 u_50 (m/s) : 8.24 Beta : 0.136 T (Degree Celsius) : 30.79 p (mbar) : 818.344 Wind-flowing-from : N Wind-flowing-to : S


Google maps view of the site


TOYOTA
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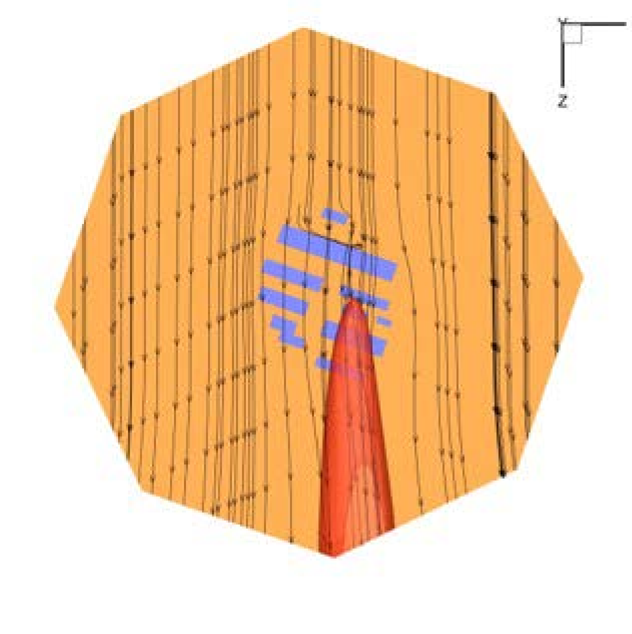
3D models for Digital twin

Conclusion and Future work



Conclusion

- Developed CFD-based framework for hydrogen dispersion modeling in both indoor and outdoor facilities.
- Integrated site-specific metadata, weather, and facility layout into a digital twin environment.
- Demonstrated how modeling informs sensor placement, detection strategies, and risk reduction.
- Established simulation pipeline as a validation platform for sensor developers and facility operators.

Future Work

- Extend digital twin to real-time integration with live sensor data and operational controls.
- Incorporate machine learning and reduced-order models for faster scenario prediction.
- Expand from steady-state to transient, multi-source leak events.
- Apply framework to diverse facilities (refueling stations, electrolyzers, indoor labs).
- Collaborate with industry partners for sensor testing.

- Thank you!
- Questions?

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