Hydrogen Emissions and Environmental Impacts Workshop
September 16-17, California, USA
Organized by the U.S. Department of Energy's Hydrogen and Fuel Cell Technologies Office in collaboration with the European Commission

Modeling of H_2 Dispersion

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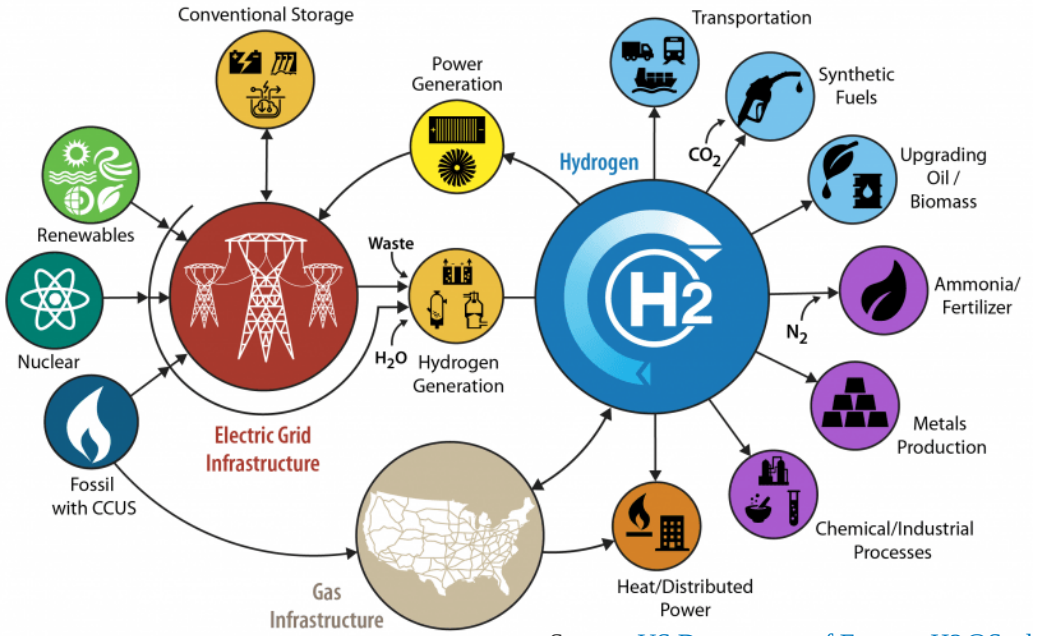
Hydrogen emissions



Source: [US Department of Energy, H2@Scale]

Important questions:

1. where does emissions go and in what concentrations? How much hydrogen was lost?
2. Where should facilities place sensors to detect leaks? How many sensors?
3. Can you do wide area monitoring for hydrogen emissions?

and more…

Hydrogen emissions monitoring

Safety

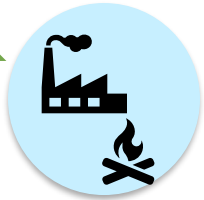
- Small scale (<100 m) monitoring
- Economic impact
- Local regulations

Environmental

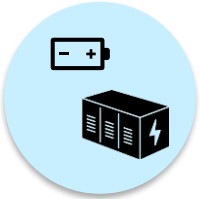
- Large scale monitoring (>100m)
- Global warming impact
- Broad environmental regulations

Aspects of sensing and monitoring

Where?



Production



Storage

Transportation

Refueling stations

How?

- Mass spectrometry
- Thermal conductivity
- Electrical conductivity
- Metal oxide sensor
- Combustible gas sensor

What?

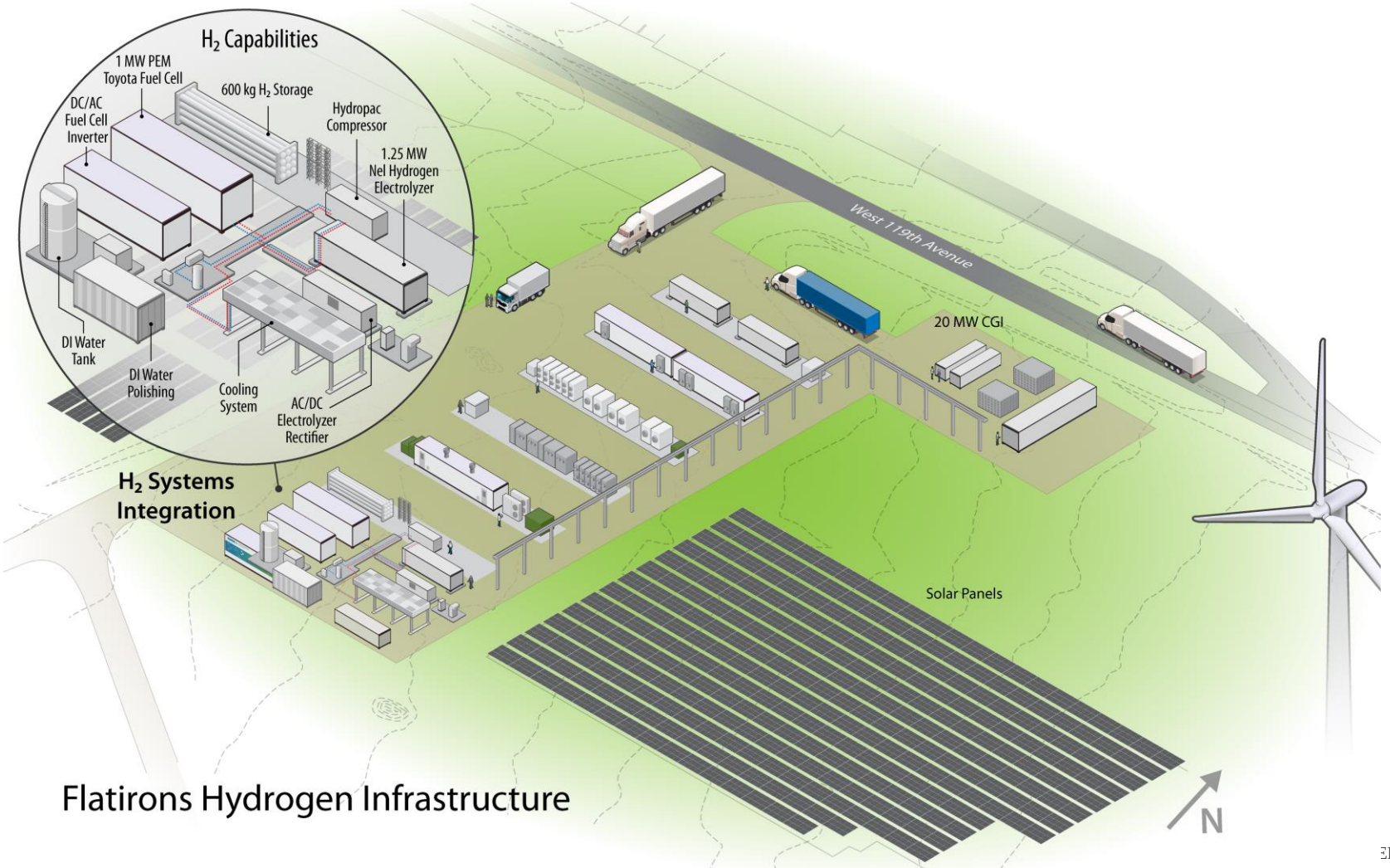
- Detection
- Measurement

- Detection and measurement strategies changes with each use case
- Economic viability, desired resolution and confidence in measurement instrument are important.

NREL Flatirons Facility

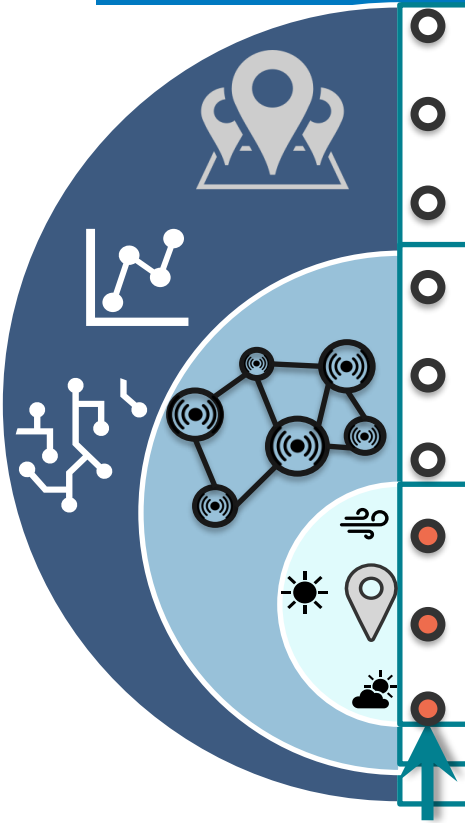
Unique site location of ARIES

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



Flatirons Hydrogen Infrastructure

Dispersion modeling - Long-term goals



Site-agnostic

- Test various site locations
- Use site specific information in predicative model
- Design a tool for recommendation of H_2 leak sensor placement

Site-optimized

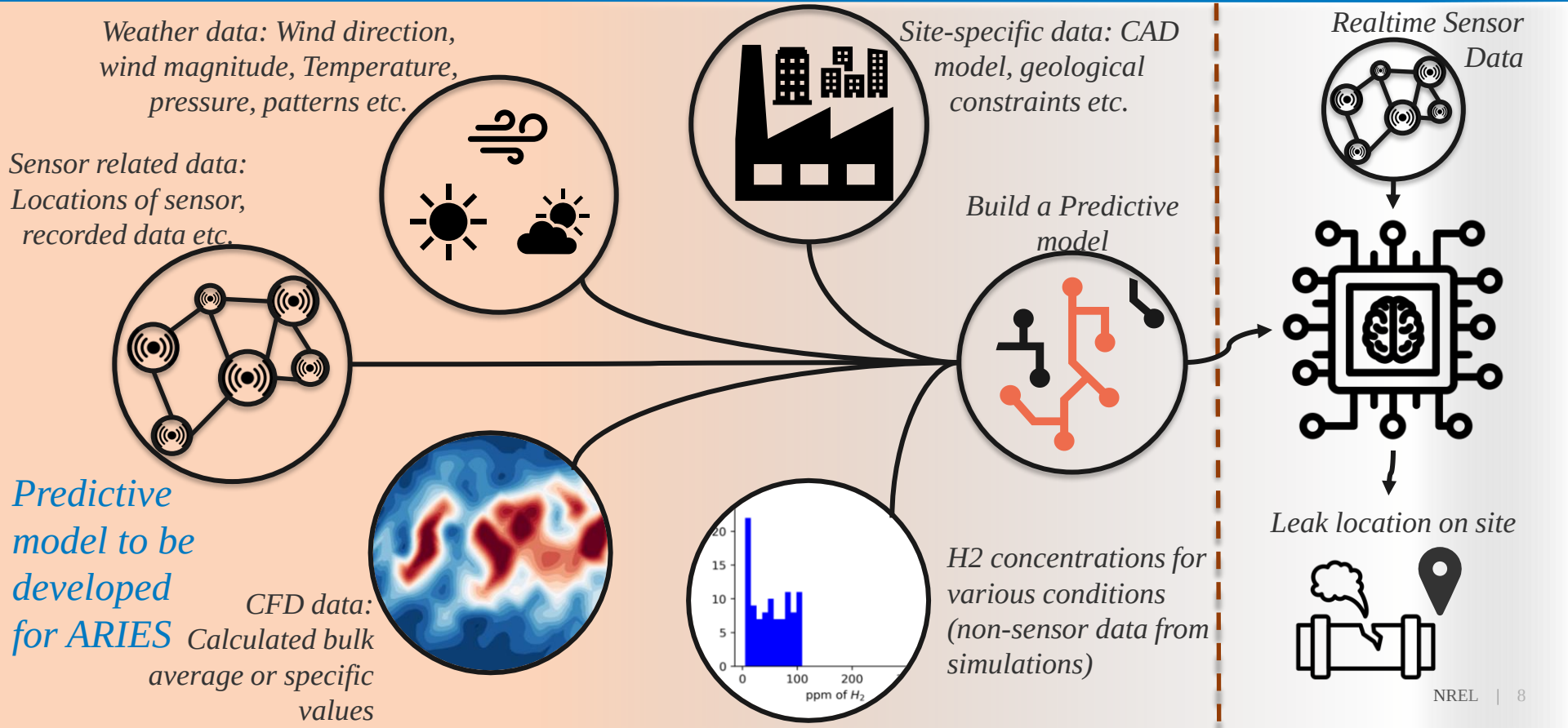
- Vary sensor locations with various site-specific conditions
- Predict leak source from H_2 concentration detected by sensors

Site-specific

- Conduct ARIES specific CFD Modeling
- Generate site specific H_2 concentration map from weather data

Three stage plan for hydrogen dispersion modeling

Hydrogen Dispersion modeling: Blocks for predictive model



Ongoing Efforts

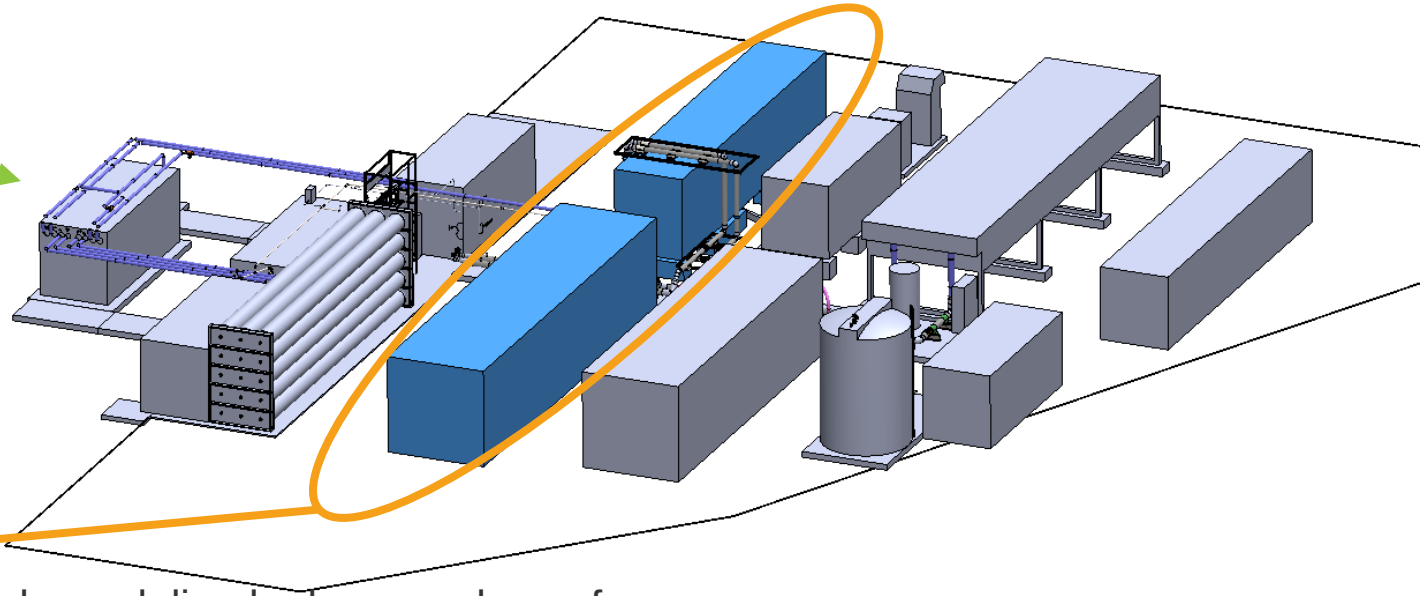
Small scale (<100 m) monitoring

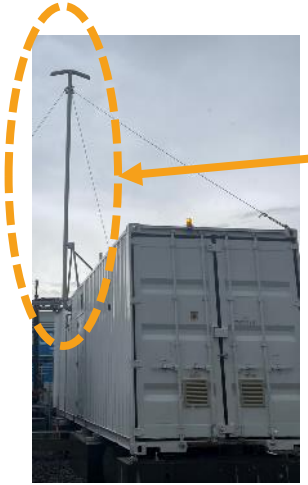
- <5 ppm
- >20000 ppm

Large scale monitoring (>100m)

- Gaseous tracer compounds (NO2,C2H6) based monitoring

Hydrogen Dipsersion modeling at ARIES





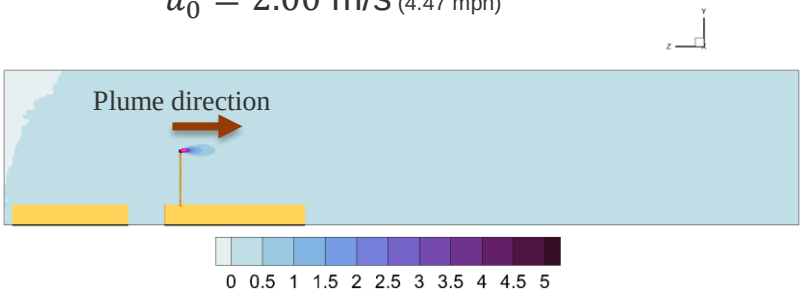
Example modeling hydrogen release from vent (dashed oval to left):

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

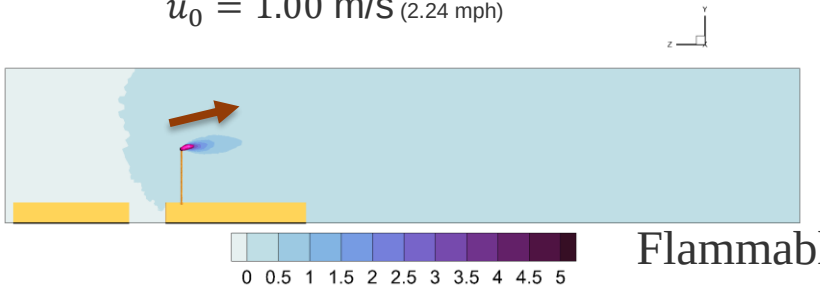
Controlled release scenarios can be performed at ARIES

H_2 dispersion behavior

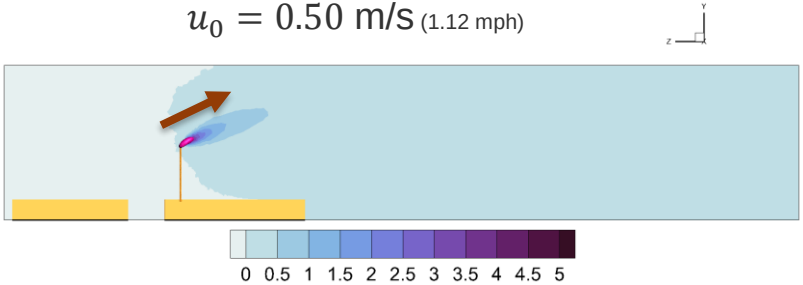
$u_0 = 2.00$ m/s (4.47 mph)



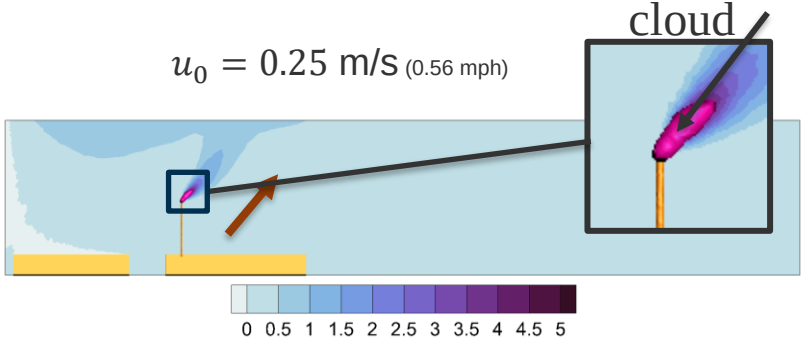
$u_0 = 1.00$ m/s (2.24 mph)



$u_0 = 0.50$ m/s (1.12 mph)



$u_0 = 0.25$ m/s (0.56 mph)

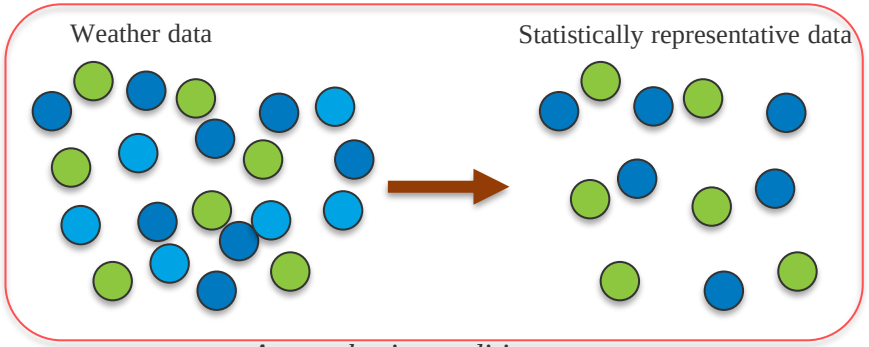


Hydrogen dispersion nature is wind dependent

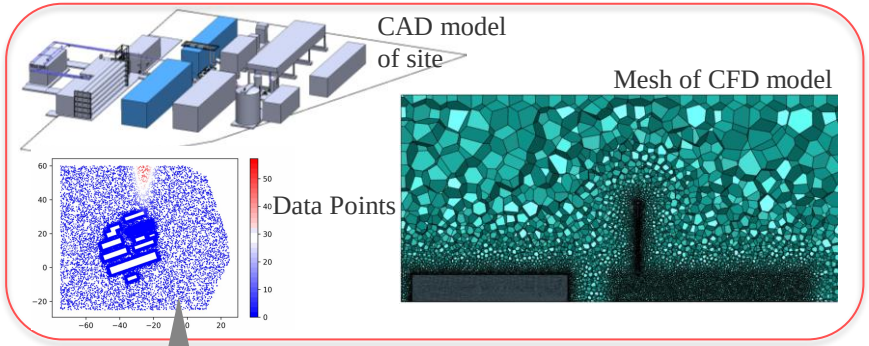
Stages of Hydrogen leak Modeling

Developed pipeline for sensor placement strategy

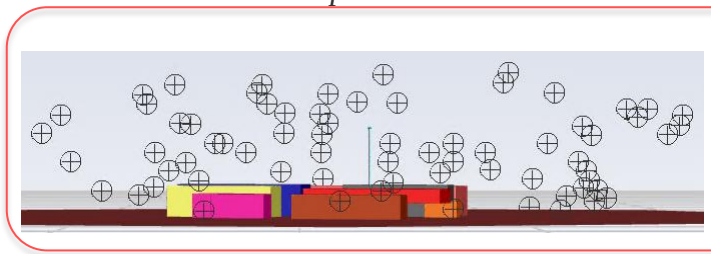
Site specific weather information → Site specific CAD and CFD modeling → Data processing of H_2 concentration → Sensor locations



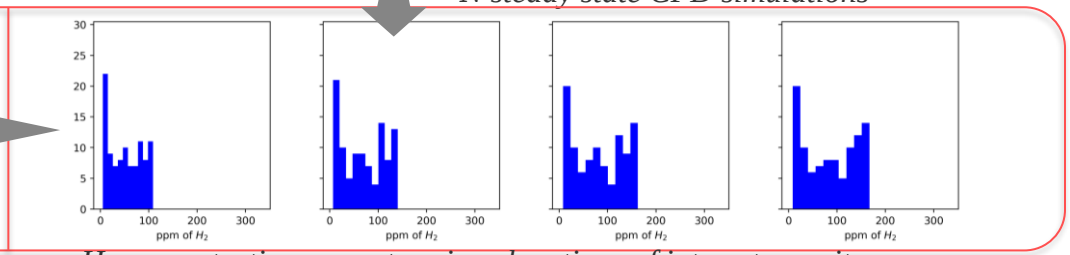
Atmospheric conditions



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

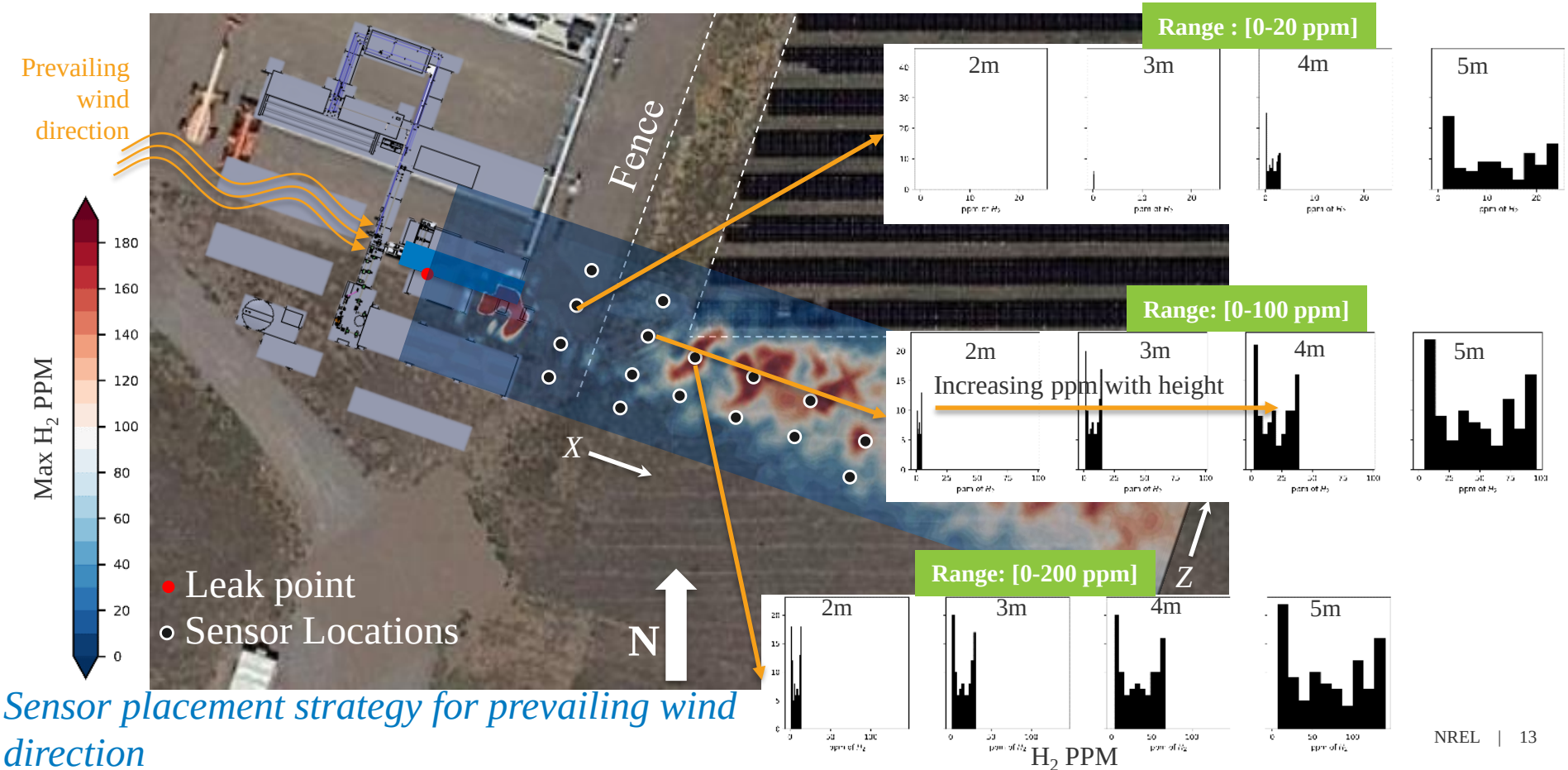


Approximate sensor map



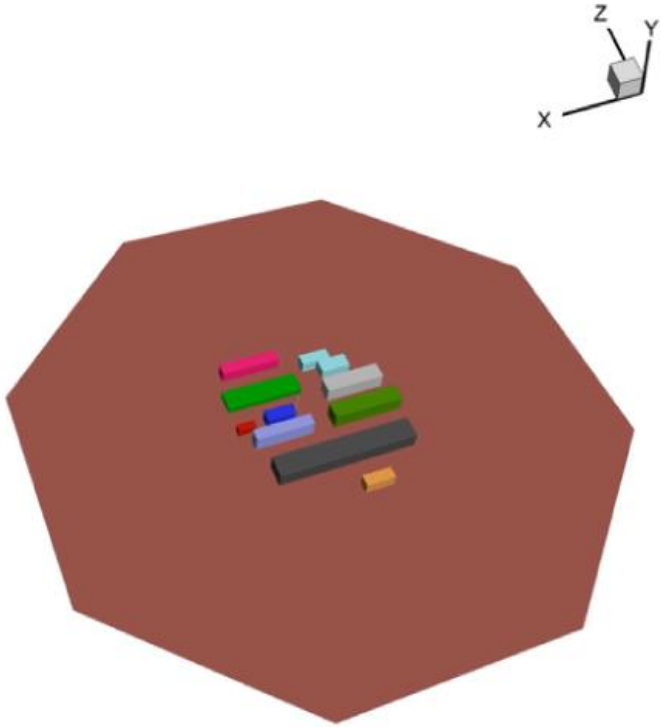
H_2 concentration map at various locations of interests on site

Hydrogen dispersion and deployment of sensors



Sensor placement strategy for prevailing wind direction

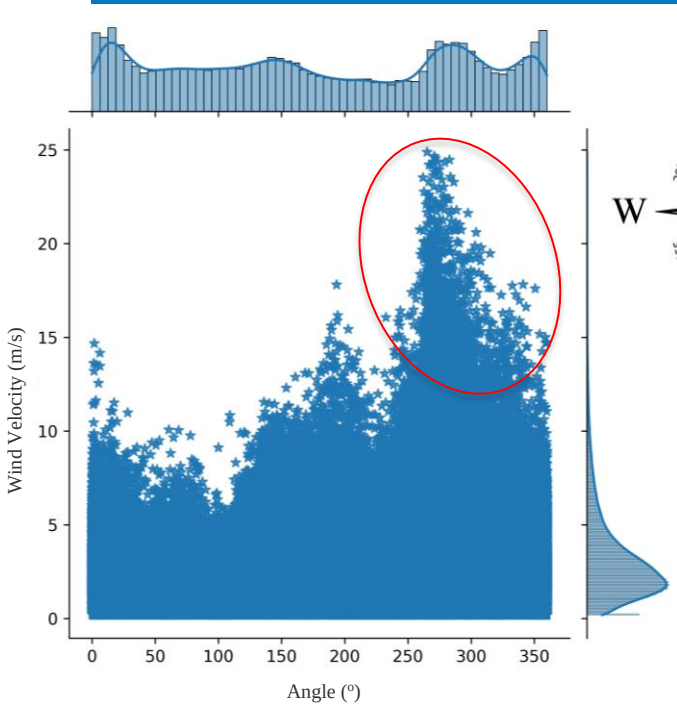
Simulation Domain

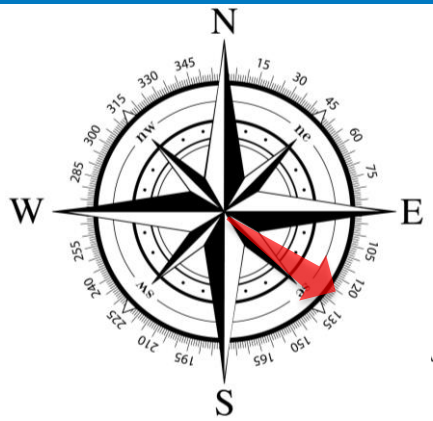


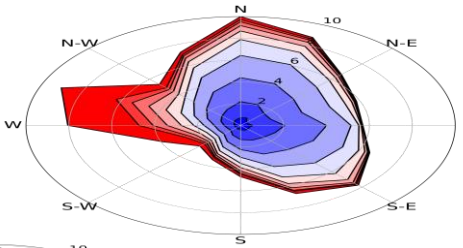
Site-specific and accurate representation of ARIES in modeling

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

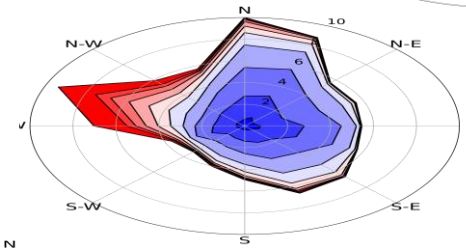
Windrose plots at various heights (2,5,10,50 m)



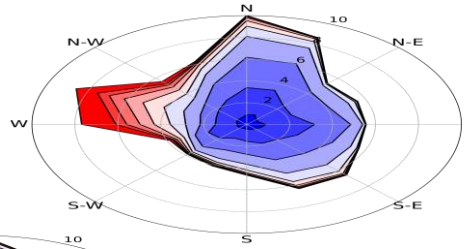




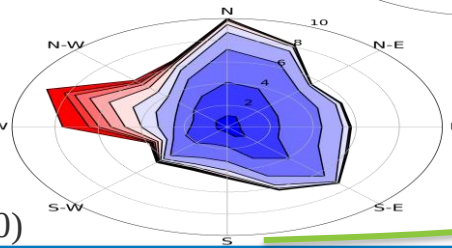
Y =50 m



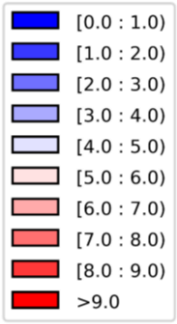
Y= 10 m



Y= 5 m



Y= 2 m

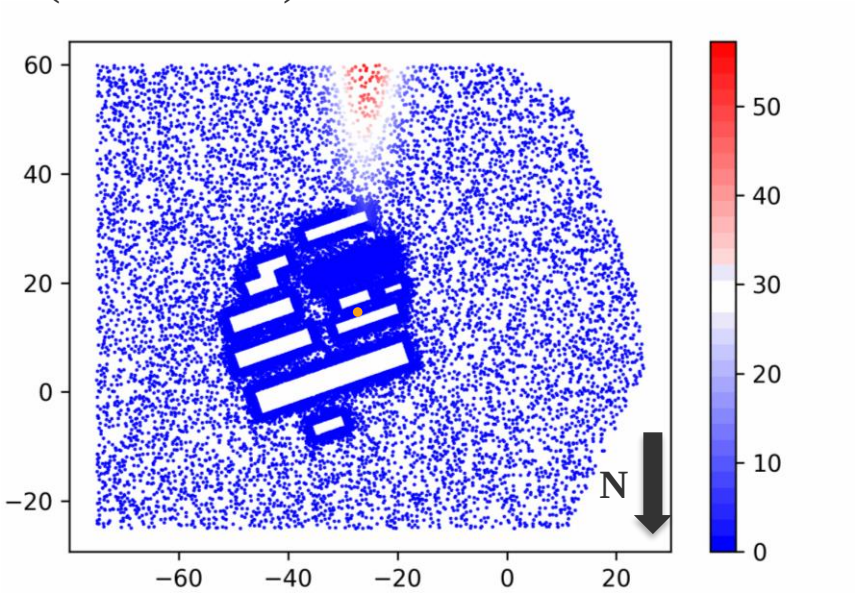


ARIES site has low to extreme wind scenarios Up to 55 MPH

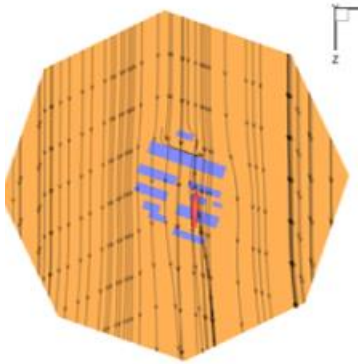
Ground (Y = 0)

CFD modeling and statical sampling

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

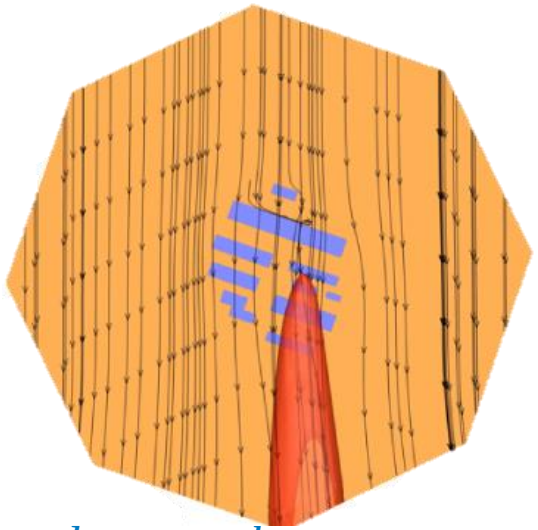


~1 M data point tracked over 240 simulations



Propagation of hydrogen cloud after leak at 26 mph of wind

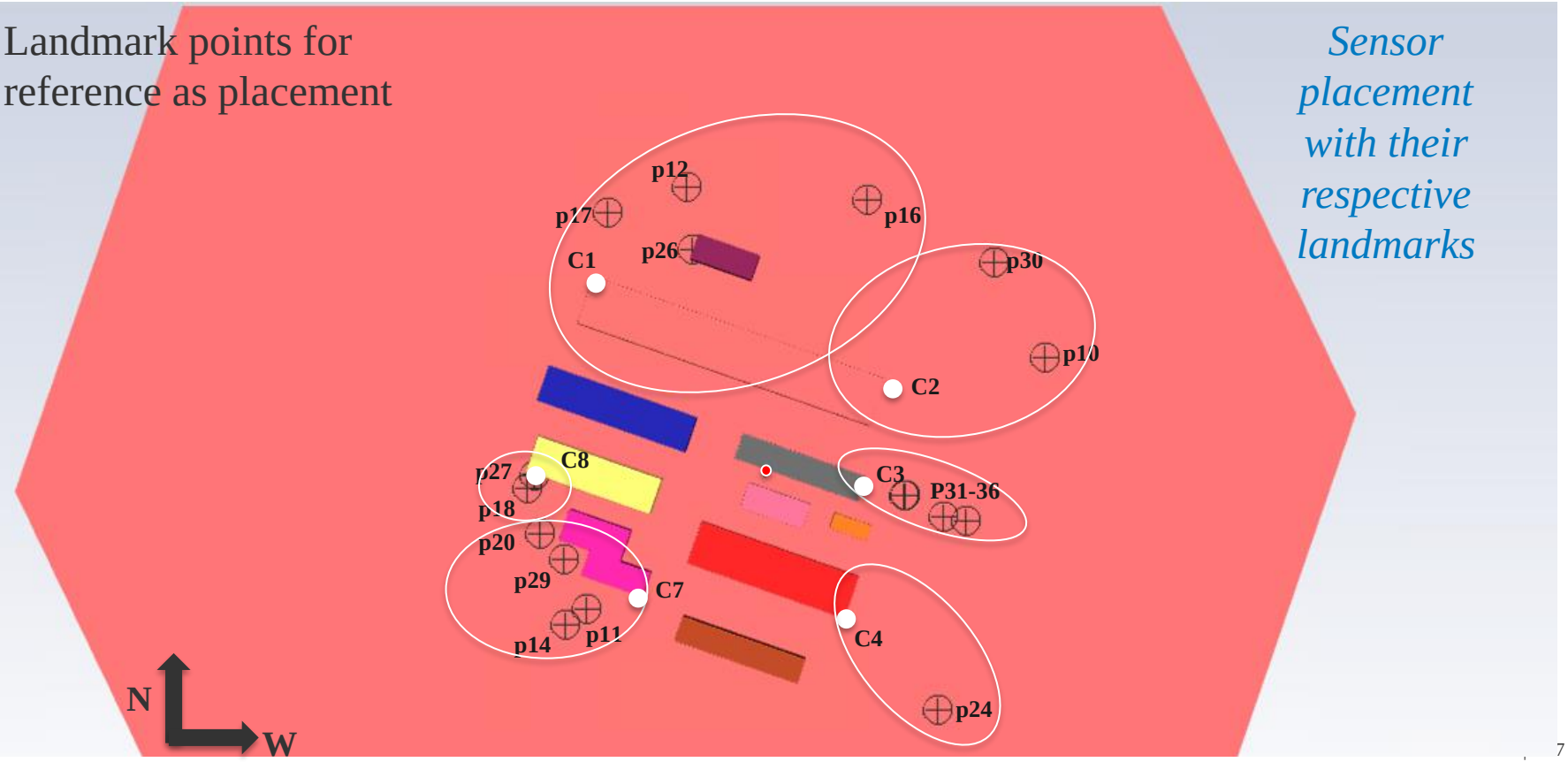
H2 leak simulation for ARIES site. Red region highlighting cloud of hydrogen above 20 ppm.



Large data ensemble and processing techniques for simulation-based approach

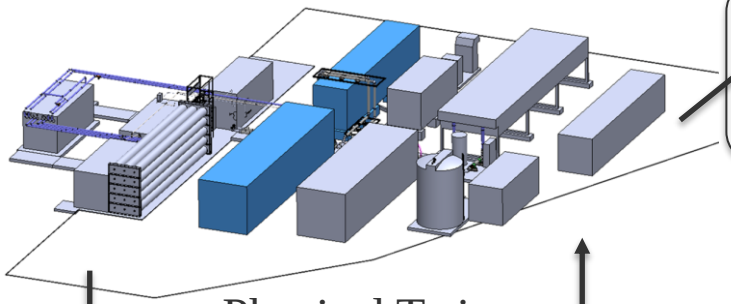
Sensor placement map- Current status of the project

- Landmark points for reference as placement



Sensor placement with their respective landmarks

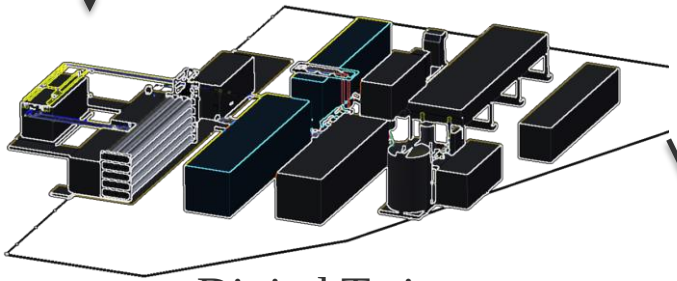
Digital Twin development
(Industry partner : GTI energy)



Physical Twin

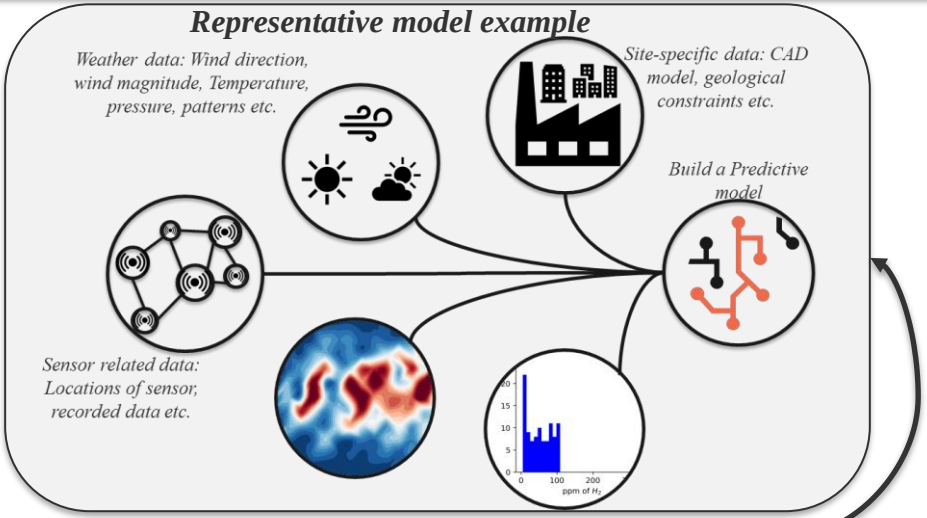
Data Collection

Information & Decisions



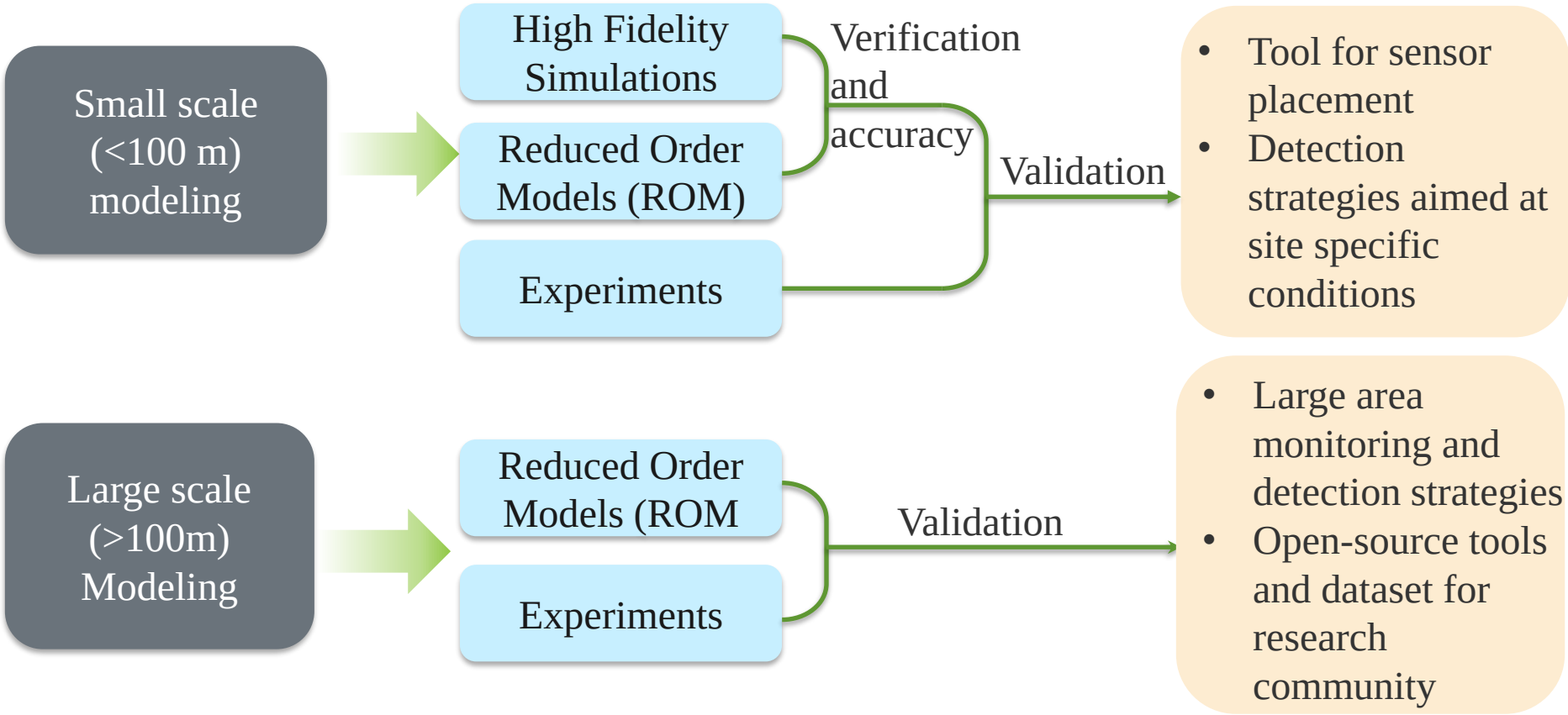
Digital Twin

- Objects (site physical data etc.)
- Processes (Leak rate, location etc)
- Various systems and conditions (e.g. Site weather data)



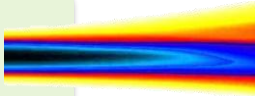
- Representative models (e.g. Predictive models)
- Data management (e.g. on demand data for users)
- Data analytics (e.g. risk factors, probability maps)

Modeling Strategy

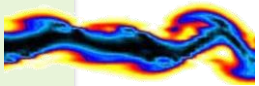


Future work and Planned activities

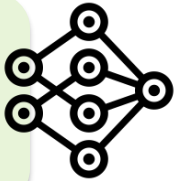
RANS based CFD simulations



High Fidelity simulations in OpenFOAM



Explore Reduced order models (ROM) for >100 m for large scale dispersion



ARIES CFD/ROM based Leak source predictor models

Develop ARIES as testbed for hydrogen sensor testing and validation

Build dataset/Digital twin to as benchmark for the other academic and partner institutions for hydrogen dispersion

Continuous improvement in analysis and modeling strategy while incorporating stakeholder engagement and interest for ARIES and hydrogen capabilities at NREL

Support for the NREL HSR&D Program is through the DOE HFTO Safety, Codes & Standards (Laura Hill, Technology Manager and Christine Watson, Technology Manager)

Specific support for modeling hydrogen releases was provided under the 2021 H2@Scale CRADA Call Supporting Advanced Research on Integrated Energy Systems (ARIES) CRADA “Next Generation Hydrogen Leak Detection--Smart Distributed Monitoring for Unintended Hydrogen Releases”

Anticipated funding: ARPA-E Funding Opportunity No. DE-FOA-0002784 “H2Sense”

For more information, contact: Munjal.Shah@NREL.GOV

www.nrel.gov

Thank You

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