O2.3-436

Subsurface to atmospheric transport of radionuclides using physics-based and machine learning models

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Lawrence Livermore National Laboratory

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Aeolus Atmospheric Simulation Tool

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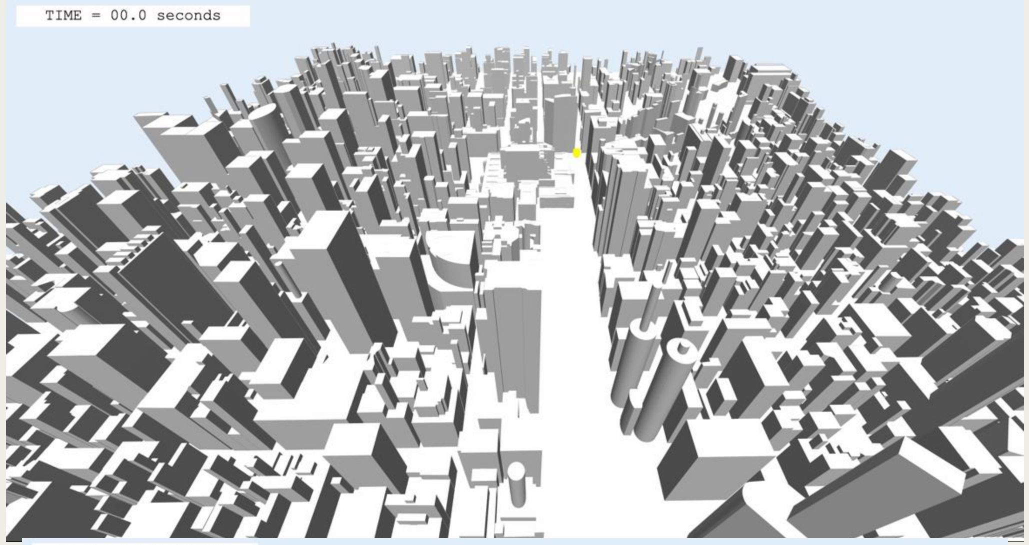

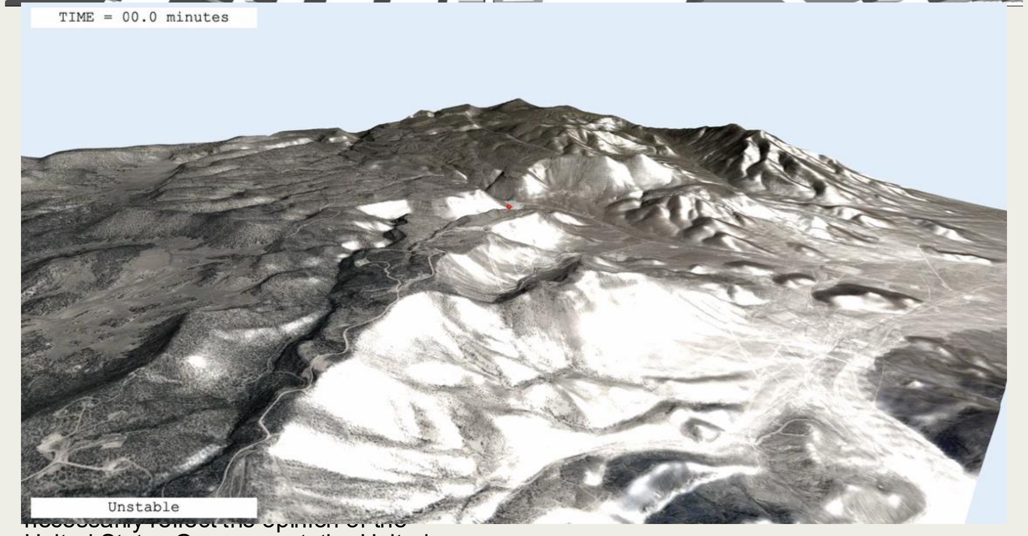

- Work done at University of Utah, Los Alamos National Laboratory and Lawrence Livermore National Laboratory has led to fast running Computational Fluid Dynamics models.
- ***Aeolus*** is an efficient three-dimensional computational fluid dynamics code based on finite volume method developed for predicting transport and dispersion of contaminants in an urban area and complex terrain. It can be run in both RANS and LES mode
- The model has a coupled Lagrangian dispersion model which can prediction dispersion of particles of different size distributions and their subsequent deposition on ground and building surfaces
- Aeolus, run in RANS mode, has been operationalized and can produce end user products in less than 30 minutes
- Different datasets integrated: meteorological fields, high resolution terrain and building, day and night population, laud use database, global soil

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Aeolus model requires minimal input to run

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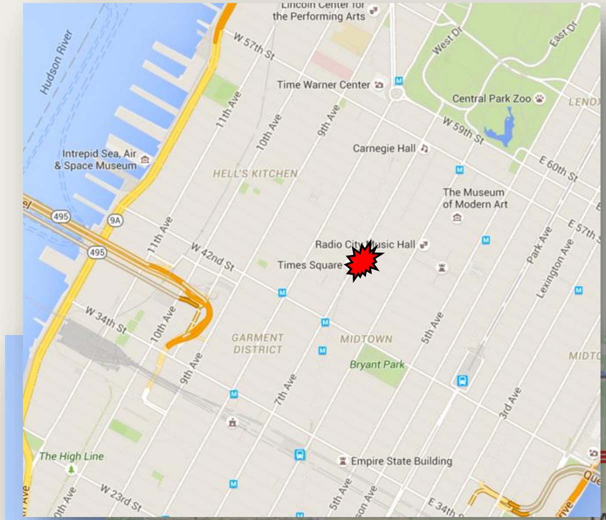
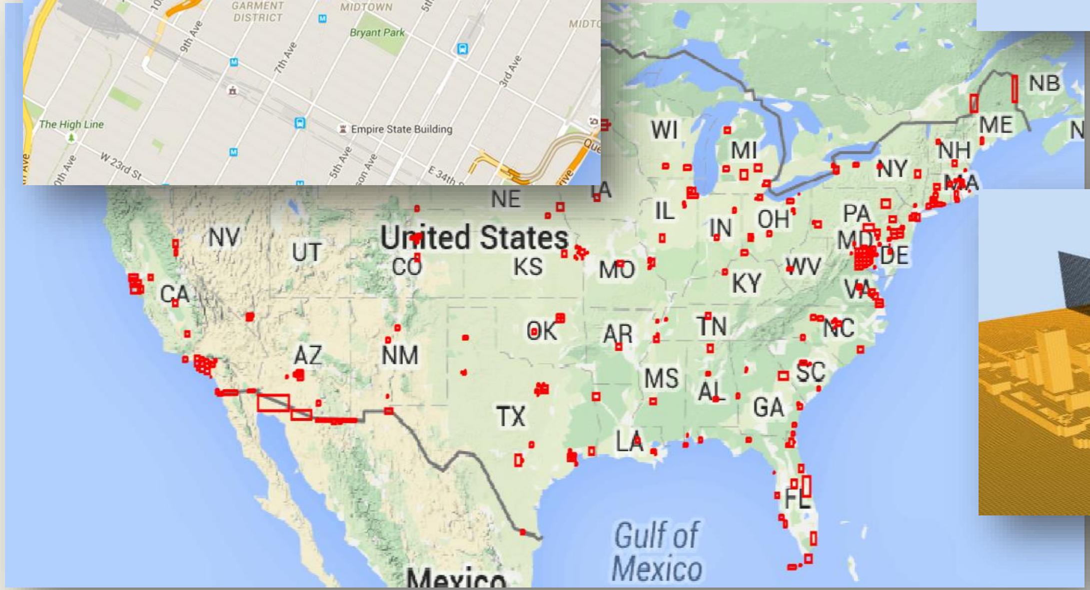
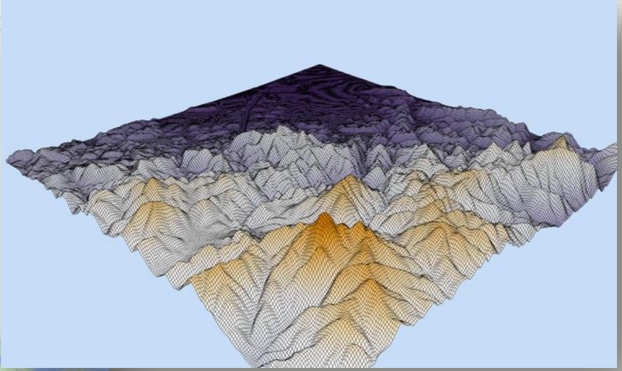
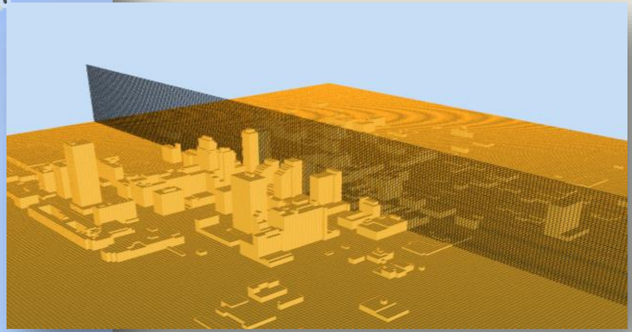
- User Input: Latitude and Longitude of the release location, Domain size, resolution, start and end time and Source characteristics
- A 3-D grid is used to model complex buildings and structures
- Model grids can be generated in seconds from GIS shapefiles (for a few kilometers) and/or building data available from a 100+ city NGA/USGS dataset
- Natural terrain elevation data is also considered when generating the grid





Terrain data (USA): Primary dataset: NED10 (**10 m resolution**; 2013 update, covers 48 states, Hawaii and portions of Alaska)





Building data: NGA/SAIC 3D building shapefiles (building footprints supplemented with height attributes). Covers most of the HSIP Gold 133 cities plus selected military and border areas

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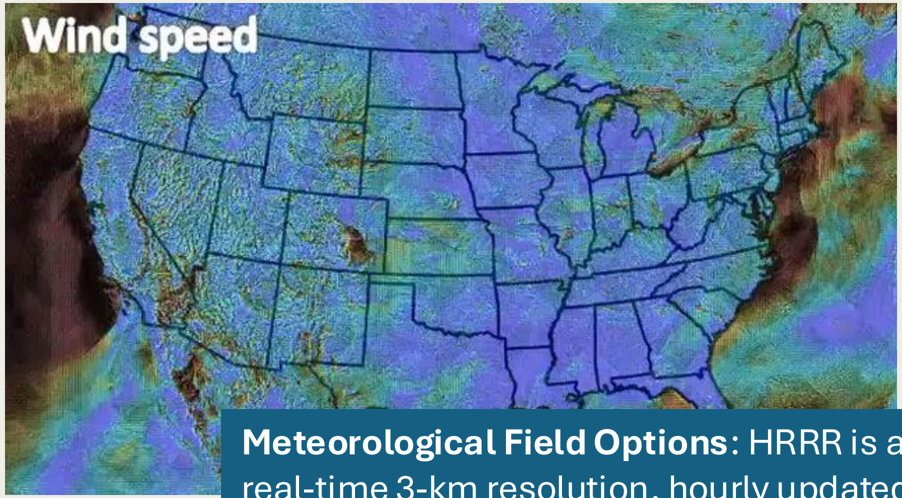
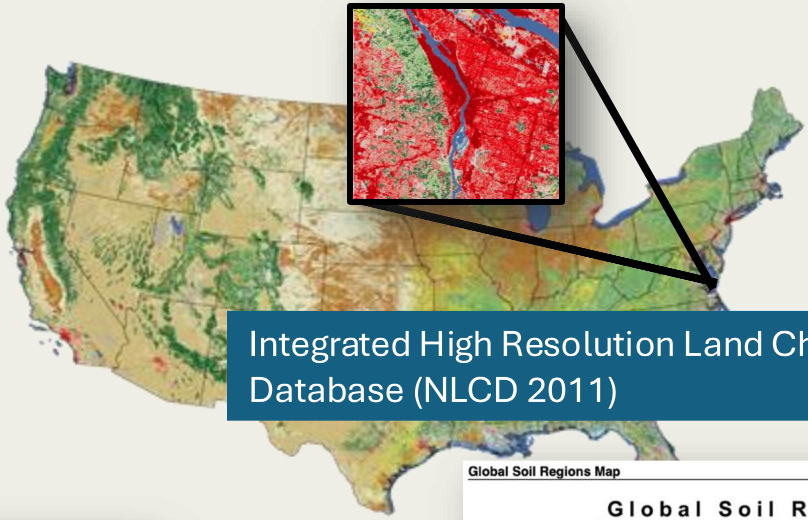
The system automatically retrieves the information needed to initialize the mode

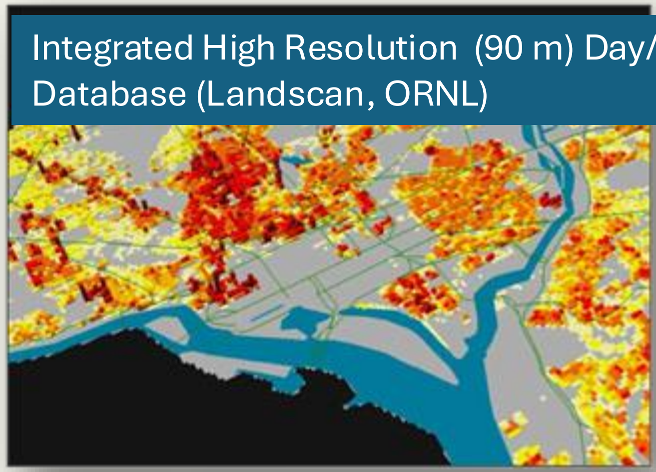


Meteorological Field Options: HRRR is a NOAA real-time 3-km resolution, hourly updated model

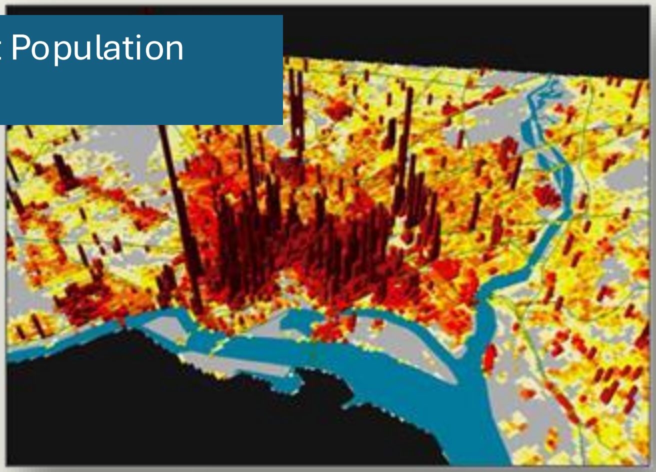


Integrated High Resolution Land Characteristics Database (NLCD 2011)

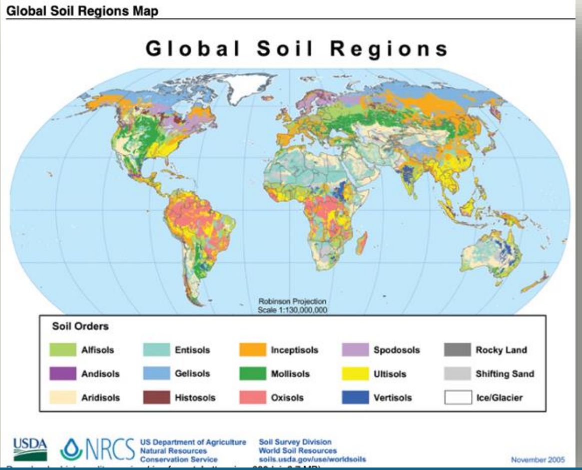
Integrated High Resolution (90 m) Day/Night Population Database (Landscan, ORNL)



Washington DC Nighttime



Washington DC Daytime



Global soil maps from Natural Resources Conservation Service Soils (USDA)

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Aeolus has been validated for predicting flow in complex terrain

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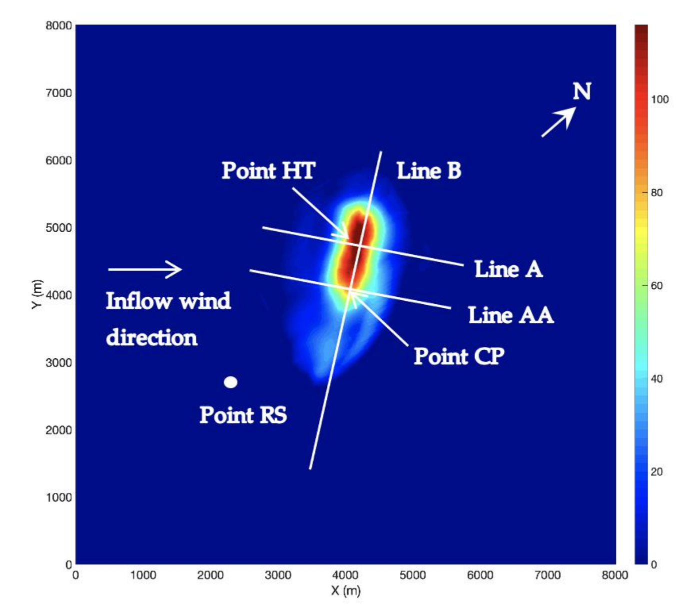

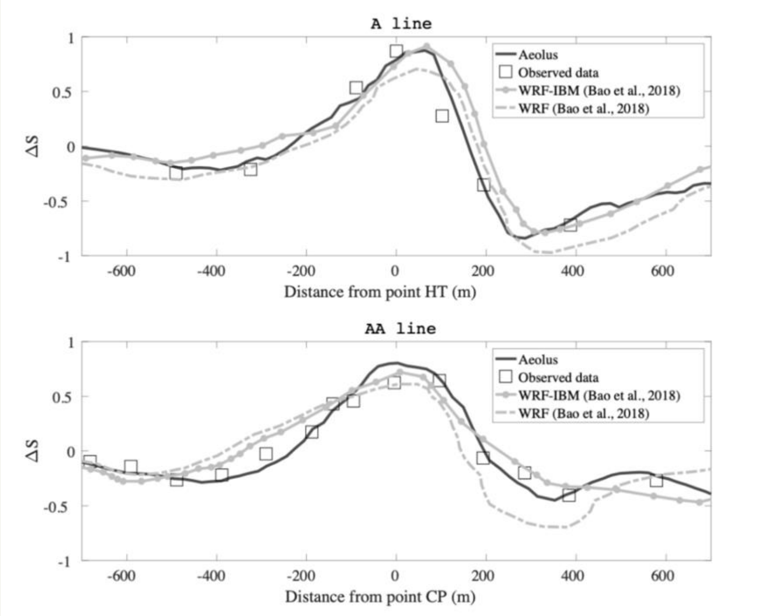

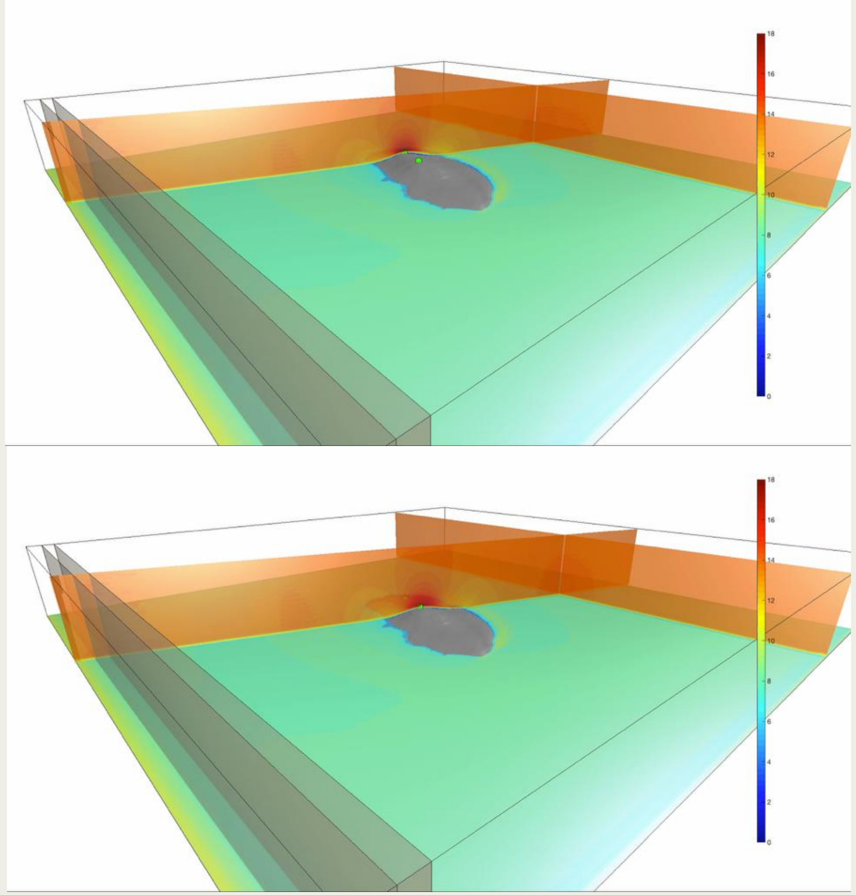

- Aeolus run in large eddy simulation mode was successfully validated using Askervein Hill dataset and the results were published in peer-reviewed journal.

Gowardhan, A.A.; McGuffin, D.L.; Lucas, D.D.; Neuscamman, S.J.; Alvarez, O.; Glascoe, L.G. Large Eddy Simulations of Turbulent and Buoyant Flows in Urban and Complex Terrain Areas Using the Aeolus Model. *Atmosphere* **2021**, *12*, 1107. https://doi.org/10.3390/atmos12091107

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REACT22 Sensors Design: Real-Time Xenon Sensors
(with Sean Stave, PNNL)

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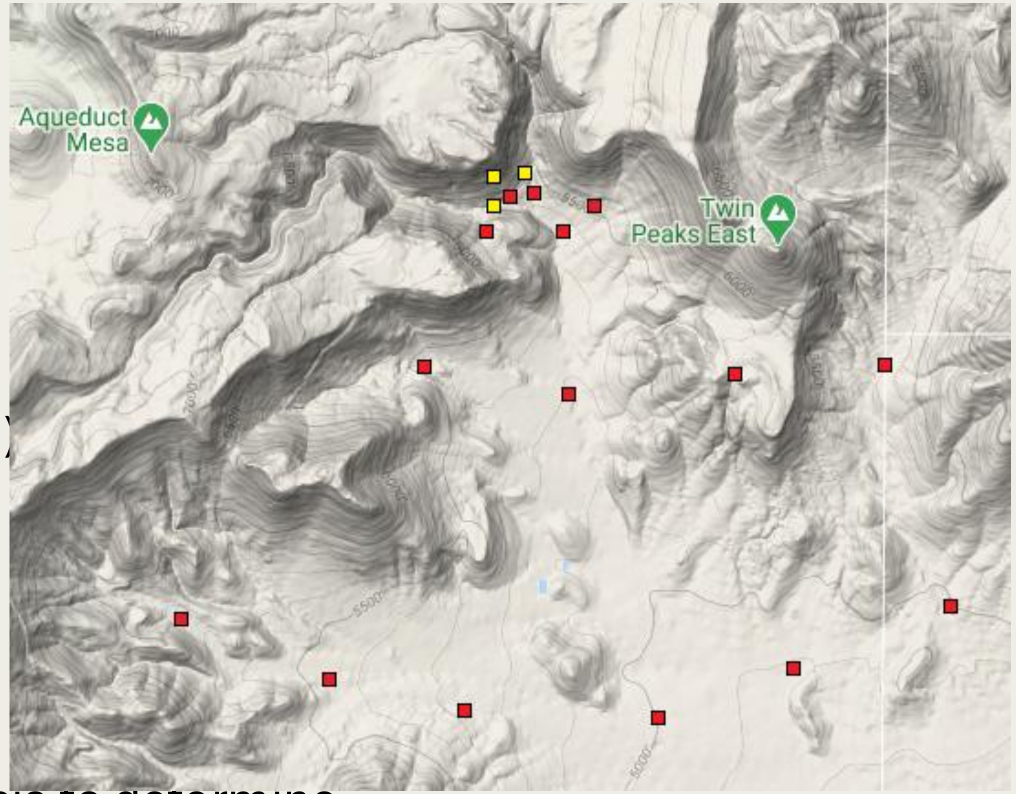
REACT22

- **Goal: optimization of detector location and release mechanisms**
  - ~5km range, but not the original 5km experiment
  - Minimal met equipment (only 10m towers), but possible evaluation of new met equipment (mini SODARs, ASSIST)
- **One week duration**
  - 6 tracer releases total, several per day possible
  - Release locations should match METREX23 plans (on apron)
  - Only release one tracer type at a time, minimal delay between the two (1 "release" = 2 tracers)
  - Evaluation of simultaneous smoke and tracer release process
- **Detector network optimization**
  - Overpopulate near-field (< 5 km), drop stations out of analysis to determine optimal density



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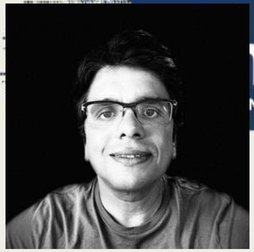

Aeolus simulation for REACT22

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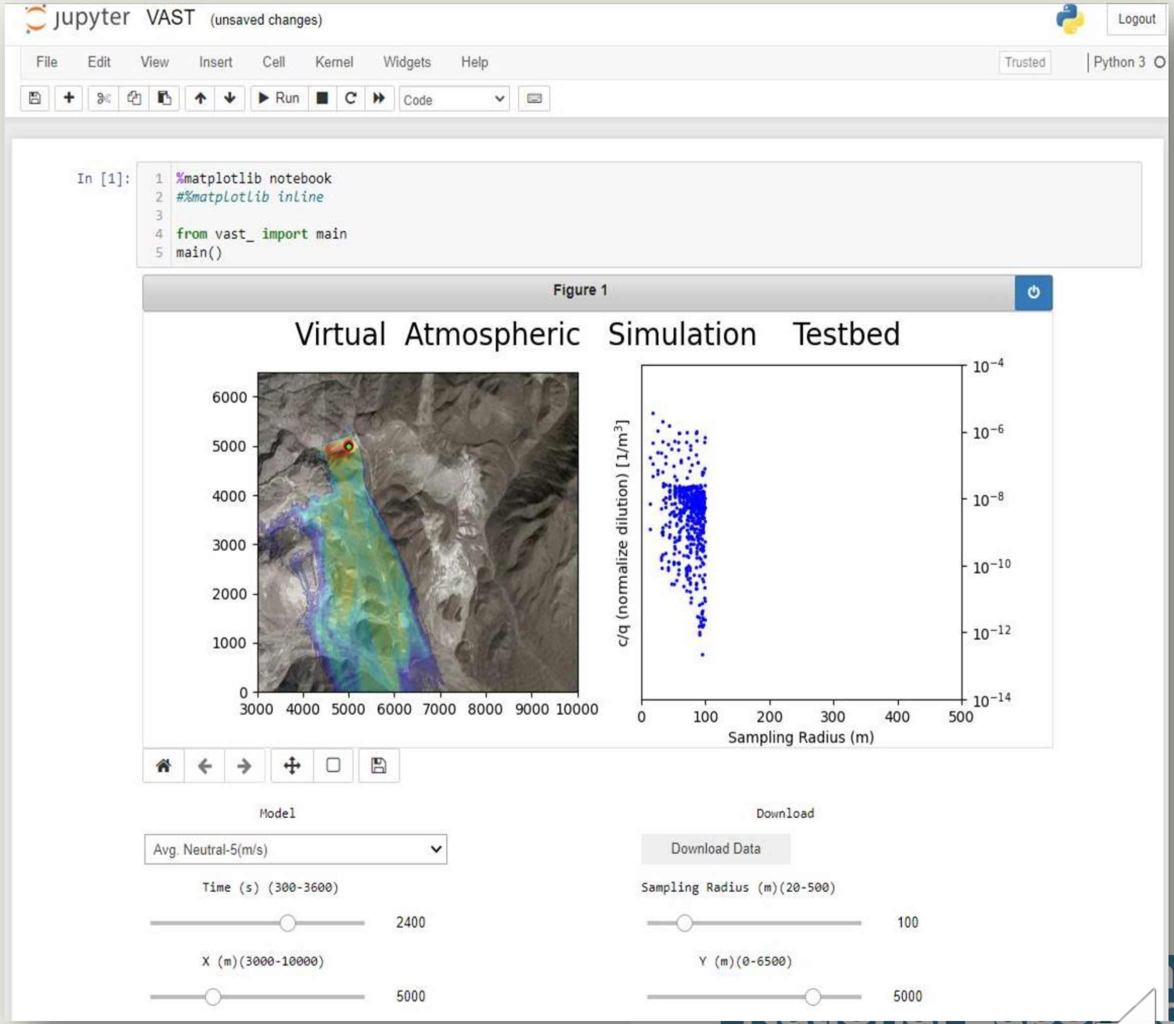
- 1 hour Aeolus simulations were performed by varying wind speed, wind directions and atmospheric stability
  - Wind direction: 330, 0 ,30
  - Wind speed : 3 m/s , 6 m/s, 10 m/s @ 10m on the mesa top
  - Atmospheric stability: Neutral
  - Two different release location
  - Release duration: 6 minutes
- 5 min average data in a sphere of 300m radius at proposed sensor locations was analyzed to determine if the sensors would be able to detect a single for these scenarios.
- A Jupyter notebook user interface was created which facilitated extraction of data at various locations



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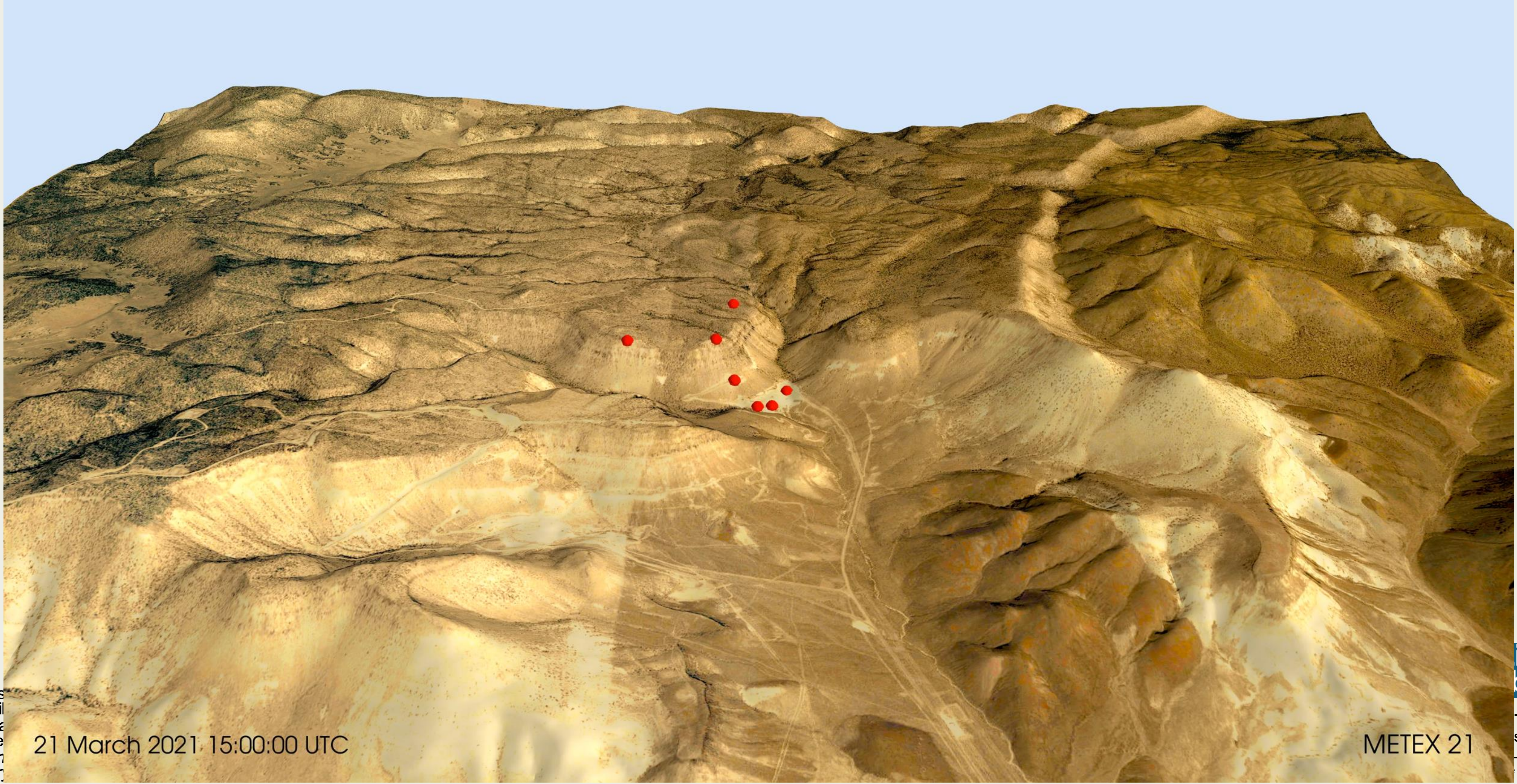

Aeolus simulation for REACT22

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Validation of Aeolus model using REACT 22 dataset

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REACT-04 Update

- Relocated 4 real-time xenon sensors and one gas sampler to closer-in positions
- Based on the offline analysis and a 5-sigma exceedance over background, observed 8 positive hits within 2 km
- Key:
  - RTXe Detect
  - RTXe + Gas Sampler* Detect
  - Non-detect

*Thanks to Ely, Bodmer and teams for Gas Sampler results

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Aeolus simulation for REACT22

Release we

Trial #	Location	WS	WD	Atmospheric Stability	PBL Height
REACT-01	Apron1	4.3	16(NNE)	Stable	100-200
REACT-02	Apron4	3.5	5(N)	Unstable	>1000
REACT-03	Apron1	4.3	6(N)	Stable	100-200
REACT-04	Apron4	6.3	6(N)	Stable	100-200

Trial• All releases occurred when apron winds were between 3 and 7 m/s and winds were northerly or north-northeasterly
• Wind speeds and direction are at tracer release point
• PBL height during release 2 is less certain because a radiosonde was not launched
• Atmospheric stability is an indication of vertical mixing strength and was estimated by the Monin-Obukhov length

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Aeolus simulation for REACT22

Initial conditions for the simulation were based on real-time data from meteorological tower MT03, located 10 meters above ground near the release site, with a wind speed of 6.3 m/s and a direction of 6 degrees. However, the model's performance was initially suboptimal compared to actual test data.

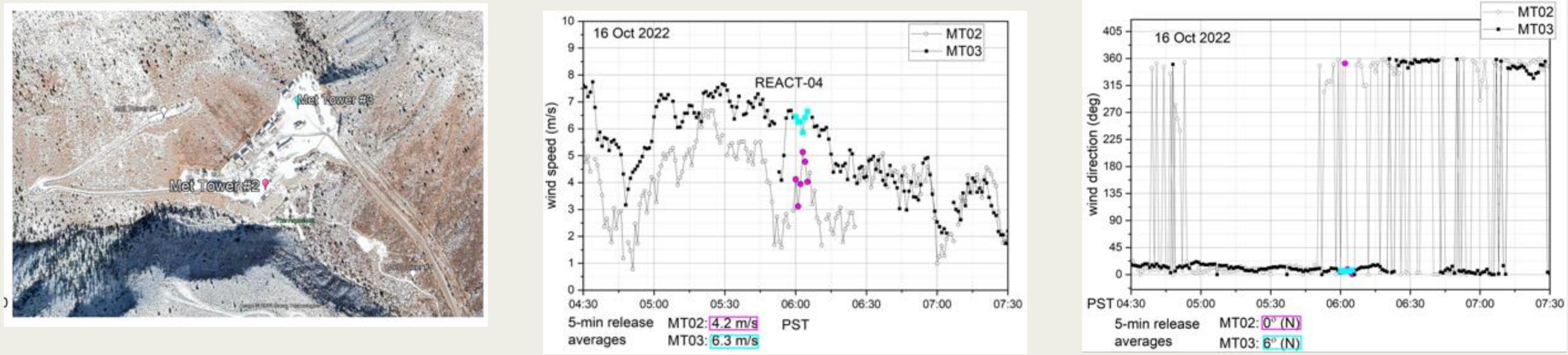

Figure 1. Meteorological tower MT03 data near the release location during REACT 04.

To improve accuracy, we reviewed data from various monitoring towers and identified tower MT01, situated on a mesa top and less influenced by surrounding terrain, as a better initialization point. This location provided more representative atmospheric conditions, free from localized effects like turbulence and wind shadowing.

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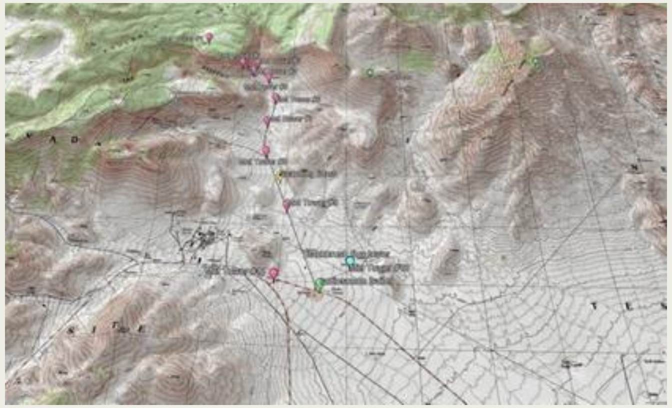
Aeolus simulation for REACT22

- After incorporating data from MT01 into the simulation, we observed significant improvements in accuracy, aligning results more closely with REACT 22 observations.
- This underscores the importance of selecting appropriate meteorological data sources for model initialization, as the quality of inflow conditions greatly affects simulation reliability.
- Future studies should focus on identifying suitable meteorological locations to enhance the accuracy of atmospheric transport models.



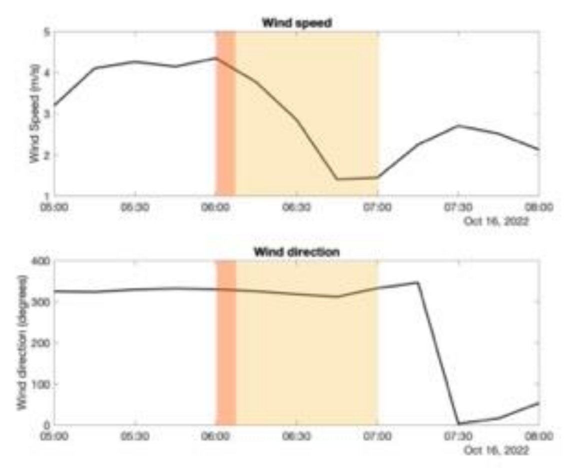


Figure 2. Meteorological tower MT01 data on the apron during REACT 04.

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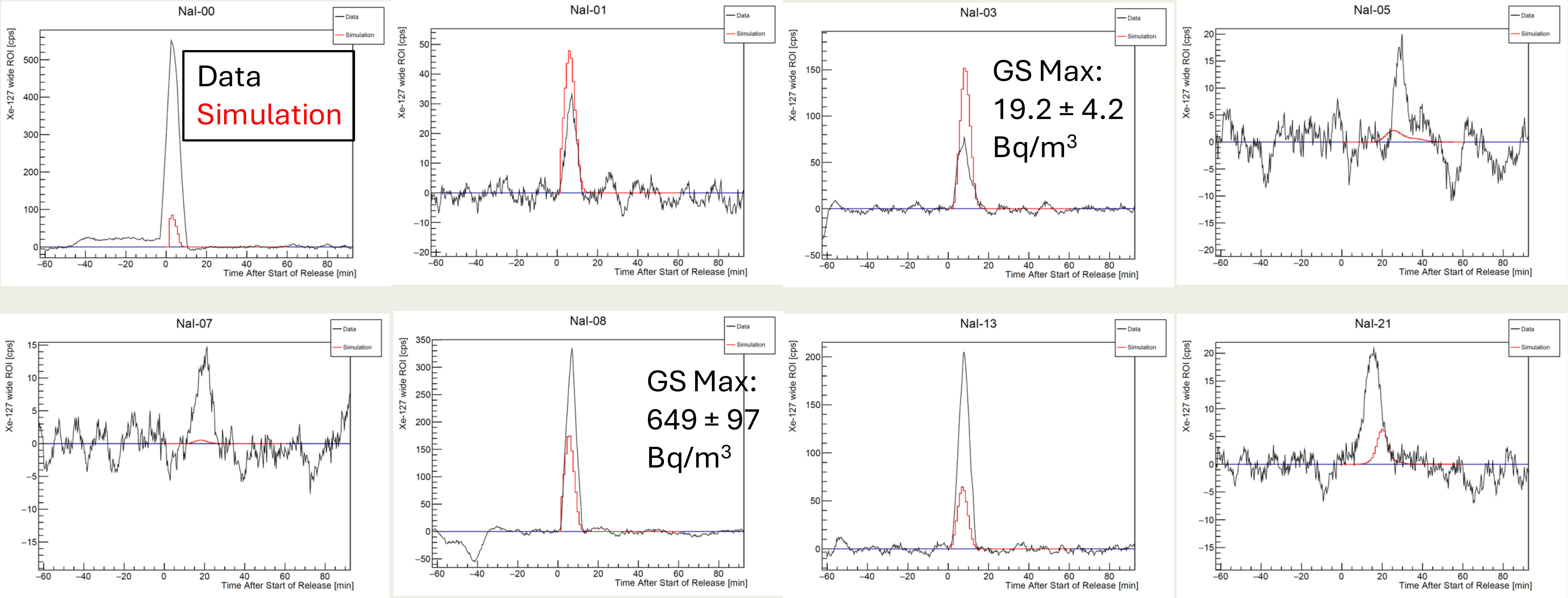
Aeolus simulation for REACT22



- For conditions: 4 m/s, wind from 350 deg, neutral
- Good timing and locations
- Some close quantitative agreement
- Gas Sample maximum results for comparison

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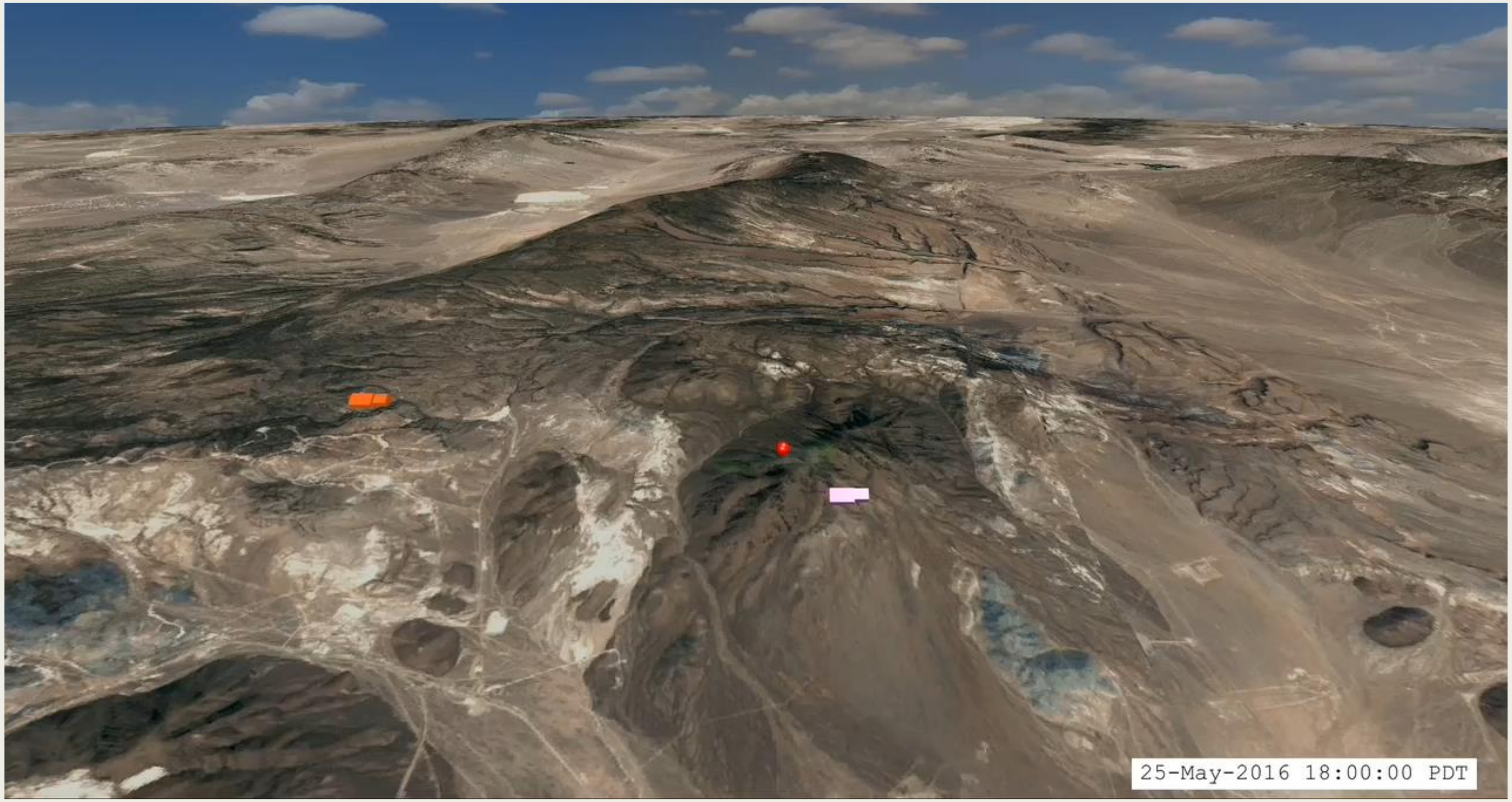
LYNM-containment: Coupling subsurface transport models to Atmospheric transport model

- Radionuclides produced from underground nuclear explosions can slowly migrate through the subsurface and vent to the atmosphere, where they are transported to detectors downwind.

- Underground test sites located in remote areas surrounded by complex terrain features can greatly affect the detectability of radionuclides once they reach the atmosphere.



We describe efforts to validate a modeling system that transports radionuclides originating from below the surface through the atmosphere using high-resolution large eddy simulations (LES) in complex terrain

LYNM-containment: Coupling subsurface transport models to Atmospheric transport model

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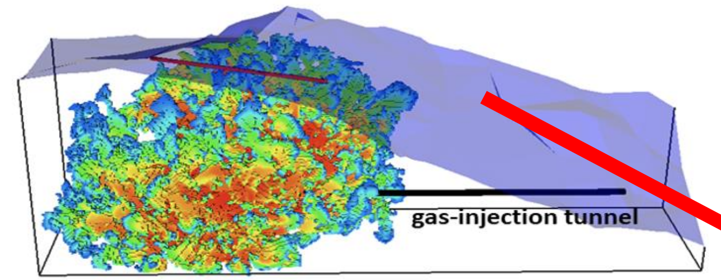
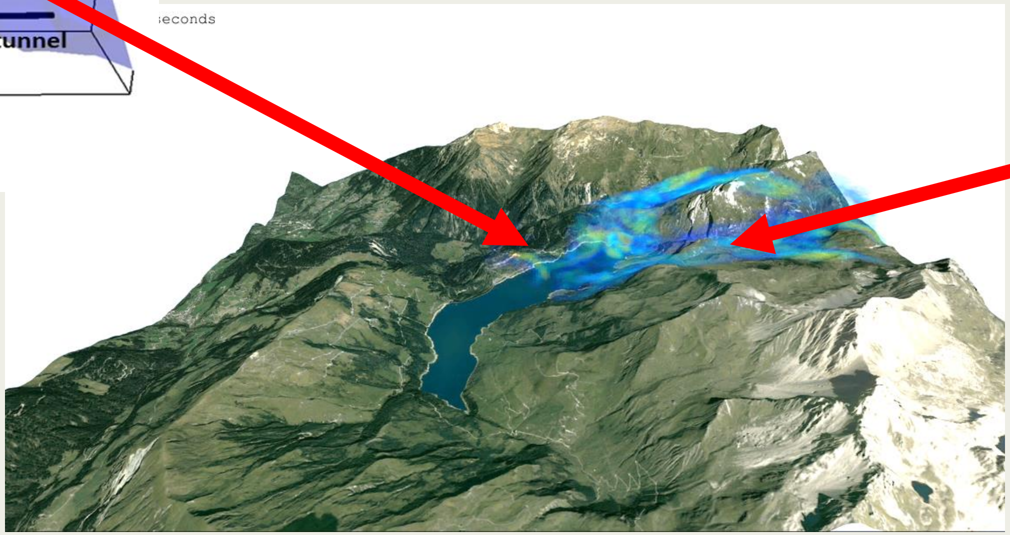
A field experiment for validating models of subsurface and atmospheric transport (SATEX = Subsurface-Atmosphere Tracer EXperiment)



Subsurface Gas Release



- Determine subsurface/atmospheric processes contributing to detection of gas signatures
- Understand uncertainties inherent in gas signatures
- Quantify confidence in detecting underground nuclear explosions
- CEA-LLNL project at Roselend Natural Laboratory, France

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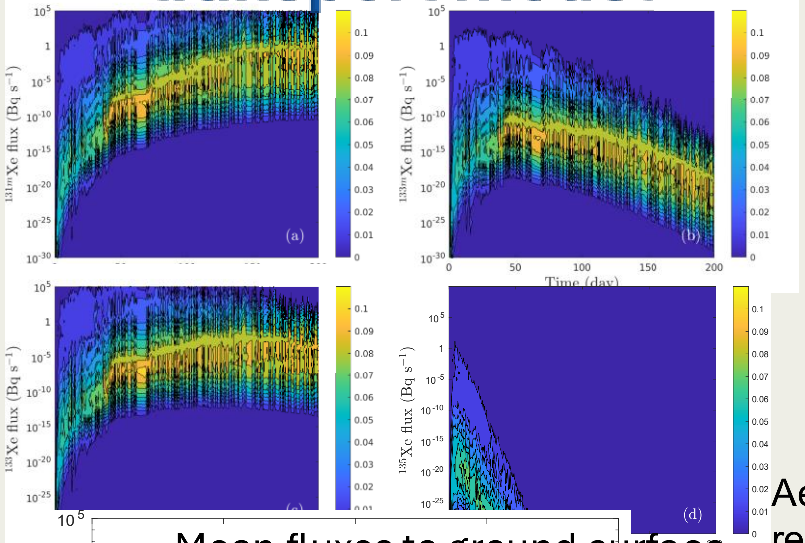
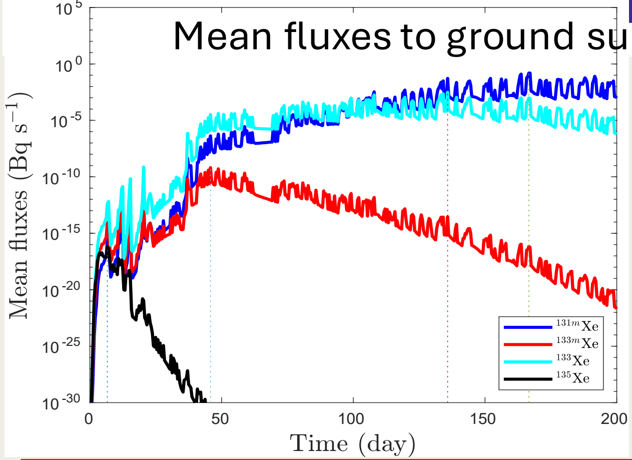
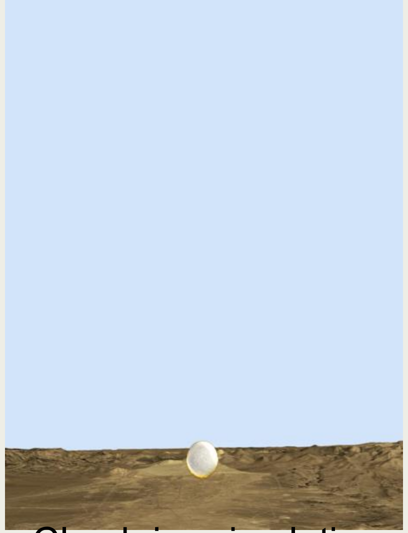
LYNM-containment: Coupling subsurface transport models to Atmospheric transport model



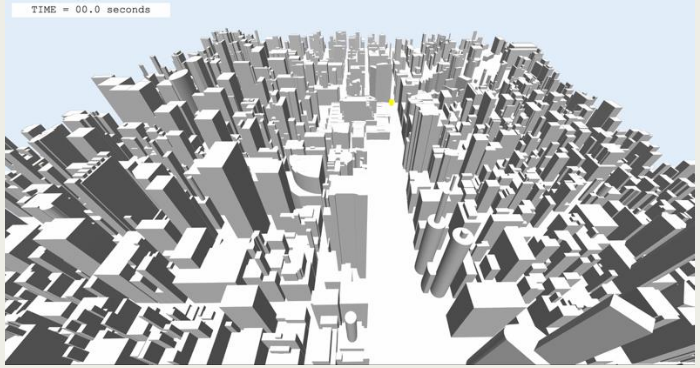


Probabilistic xenon fluxes generated from subsurface transport models serves as source terms of atmospheric transport

Aeolus simulation of radionuclide transport in complex terrain regions



Cloud rise simulation (Dixie test)



Aeolus simulation of radionuclide transport in urban areas

Lawrence Livermore National Laboratory's ***Aeolus*** is an efficient three-dimensional computational fluid dynamics code based on finite volume method developed for predicting transport and dispersion of contaminants in a urban areas and complex terrain.

NUFT is a versatile numerical model for simulating flow and reactive transport in porous media.

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LYNM-containment: Coupling subsurface transport models to Atmospheric transport model

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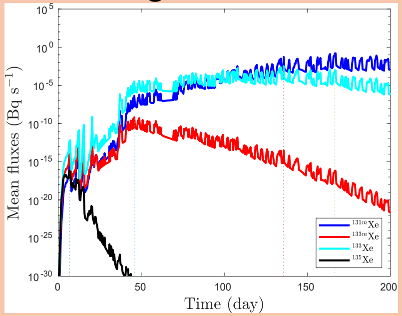
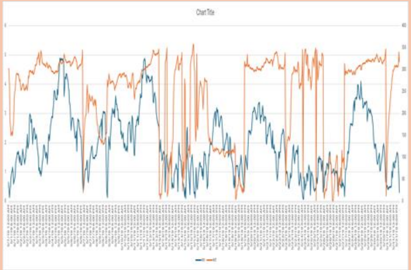
INPUT

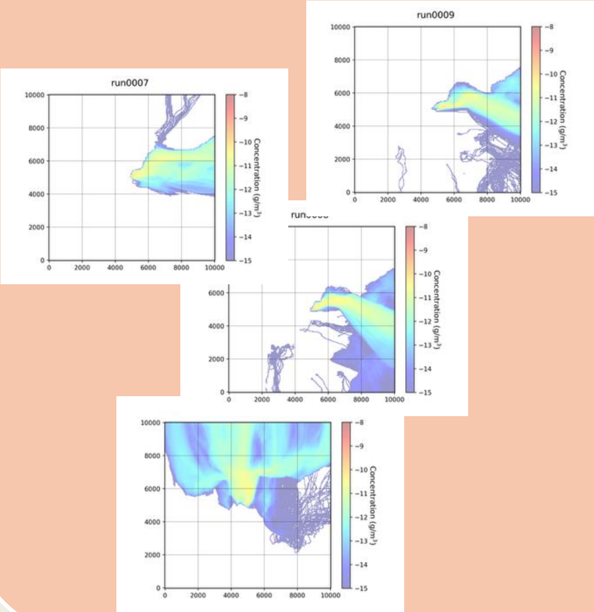
NUFT model output: Mean fluxes to ground surface



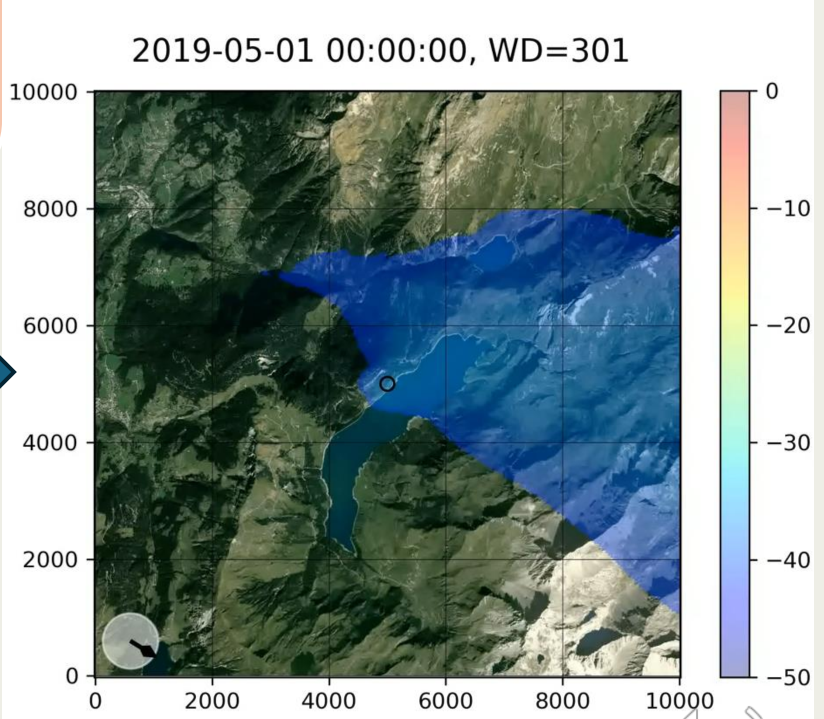
Hourly meteorological conditions



AEOLUS ensembles (~2000)



ML module



Machine learning model output

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Conclusions

- Aeolus Large eddy simulation model was used successfully for REACT22 Sensors Design.
- After the successful completion of REACT 22 experiments, the field data was used to validate the Aeolus model.
- The conventional understanding was to use the meteorological condition at the source location to initialize the atmospheric model.However, in the cases where the release scenario is situated with complex terrain feature, this can lead to suboptimal performance of the model.
- Meteorological condition should be chosen from a location which is close to the source but free from any substantial terrain influence.
- A Machine learning module was developed which can rapidly simulate atmospheric dispersion of radionuclides arising from an UNE by coupling Aeolus with output from a subsurface transport model NUFT

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