Comparison of dense gas models at different fidelity levels with experimental data

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Outline

- Dense gas dispersion
- Dense gas modeling:
  - Empirical model
  - Shallow water model
  - RANS model
  - LES model
- Validation case: Thorney Island, Trial 26
- Comparison of different models
- Conclusions

Dense Gas Dispersion

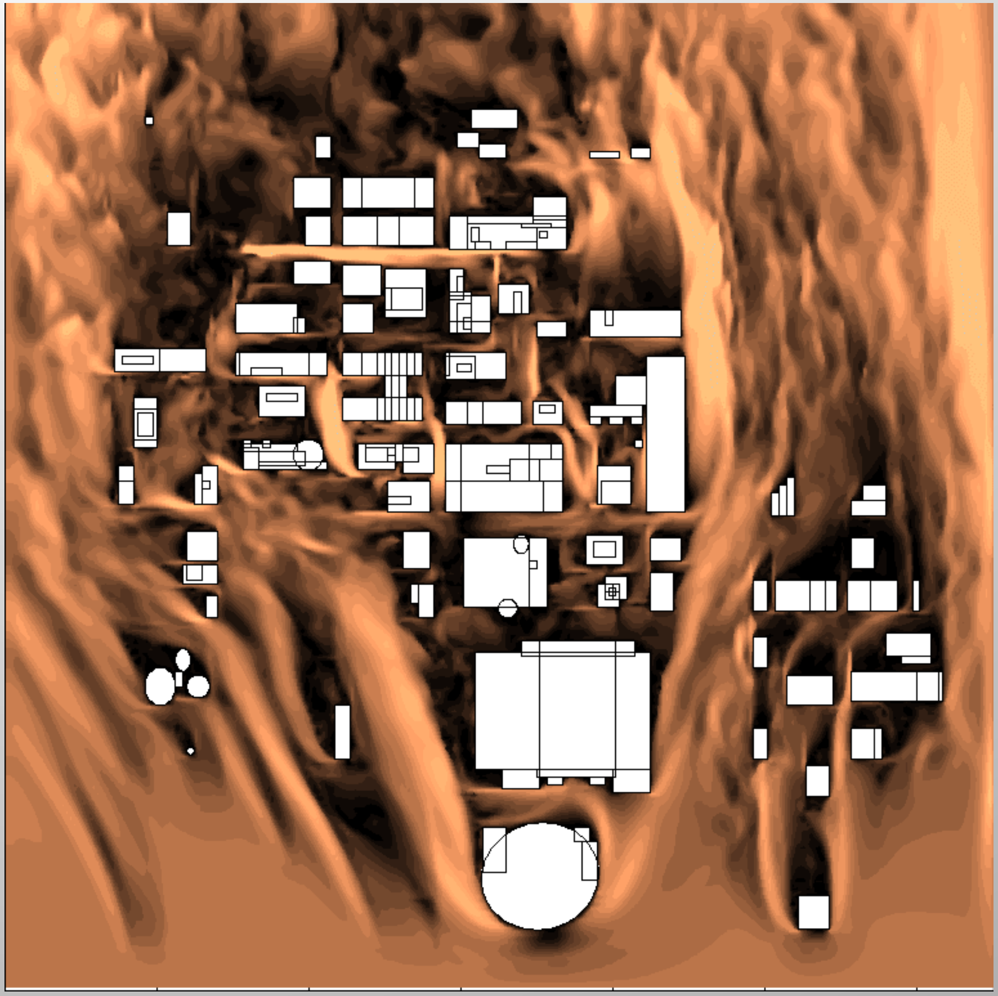
- **Huge amounts of harmful chemicals are stored and transported across the country**
- **Many of these chemicals are heavier than air or show dense gas behavior due to cold temperatures at which they are stored**
- **In the case of an accidental or deliberate release, it is important to predict the dispersion of such chemicals in the atmosphere.**
- **Due to the heavier-than-air behavior of these chemicals, they tend to accumulate near the ground, thus increasing the concentration at breathing height.**
- **The hazard zone coverage area for these chemicals tends to be larger because of slumping effect.**

Dense Gas Dispersion Modeling

- A number of empirical models have been developed to predict the dispersion of dense gas releases over flat terrain.
- However for release in an urban area or over complex terrain, these models are not sufficient.
- Computational fluid dynamics have been successfully used to predict such scenarios
- As a part of this presentation, results from two different dense gas CFD models will be compared with available experimental data. The models:
  - Reynolds Averaged Navier Stokes Model
  - Large Eddy simulation model

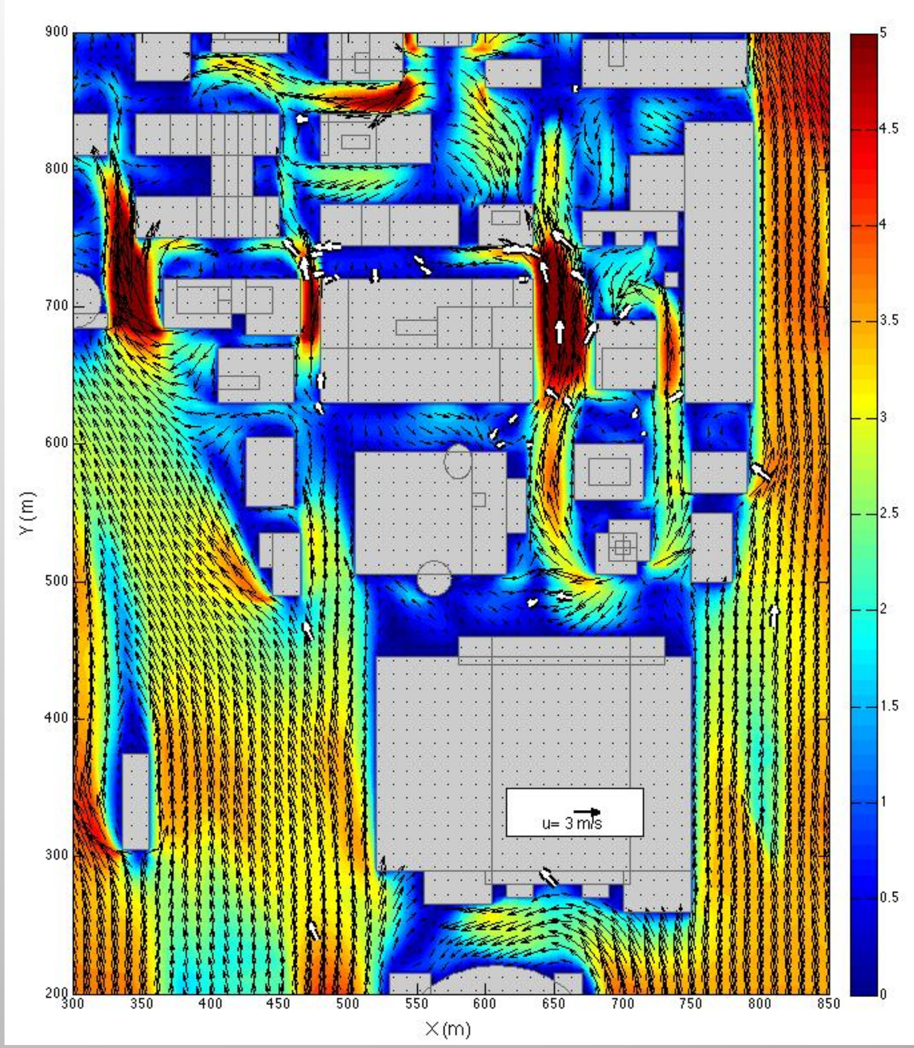
Large Eddy Simulation model

- Solves unsteady incompressible filtered NS equations
- Second order accurate in space and time
- Pressure Poisson equation solved efficiently using multigrid technique
- Log-law used at solid surface
- Smagorinsky closure



Reynolds Averaged NS model

- Solves time dependent incompressible RANS equations very quickly
- Based on artificial compressibility method (Chorin 1967)
- Uses very simplified algebraic turbulence model based on Prandtl's mixing-length theory
- Grid generation is done in seconds using existing ESRI shape files
- Runs in minutes, however, for dense gas simulation, it needs to be run in unsteady mode, which makes it computational cost similar to LES



Thorney Island Experiment

- Heavier-than-air outdoor releases
- Conducted at Thorney Island, UK 1982-1984
- Better understand dense gas behavior
- Develop and test dense gas models

Courtesy of Thomas Dunn (SAIC); photos originally from Jim McQuaid

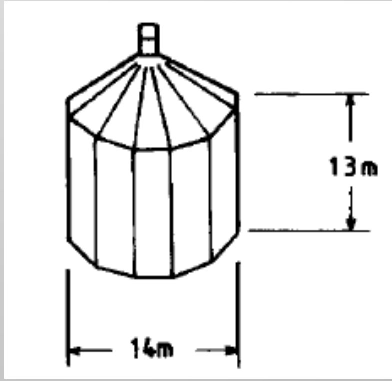
Thorney Island Experiment Trial 26

- **2000 m^3 of gas was released in about 1.5 s.**
- **The smoke marking of the gas was achieved by firing of smoke grenades.**

McQuaid, 1985b

Gas filled container before the release

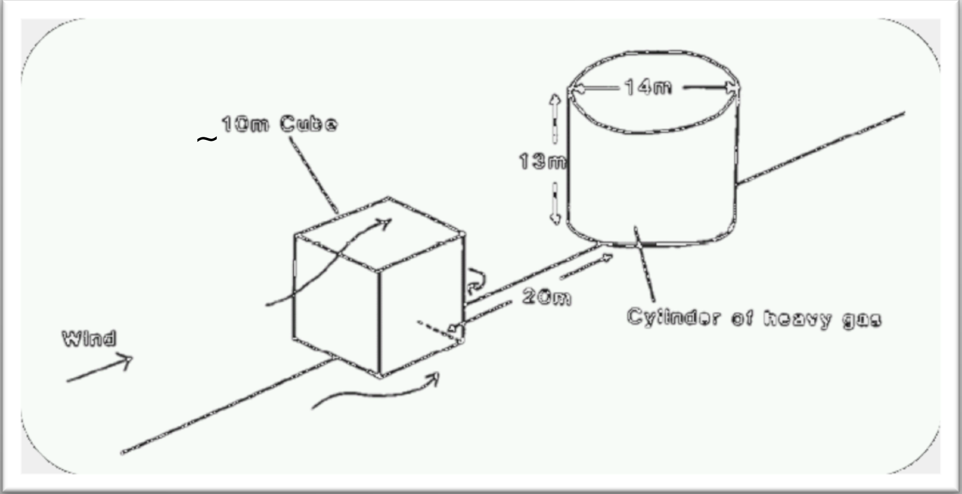
Cloud of heavy gas after the removal of the container



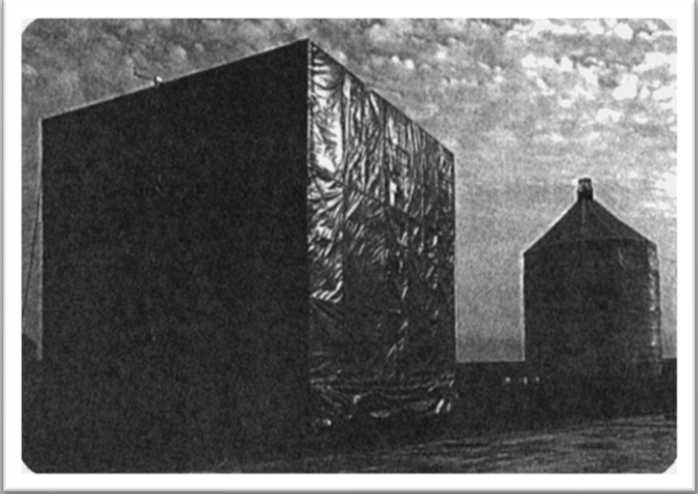
Hall and Waters (1985)

Thorney Island Experiment Phase II, Trial 26

- Investigation of the flow and dispersion in the vicinity of an isolated building
- 9 m high building 50 m downwind
- Wind speed 1.9 m/s at 10 m AGL
- Concentration samplers at 6.4 m AGL on the windward face and 0.4 m AGL on the leeward face

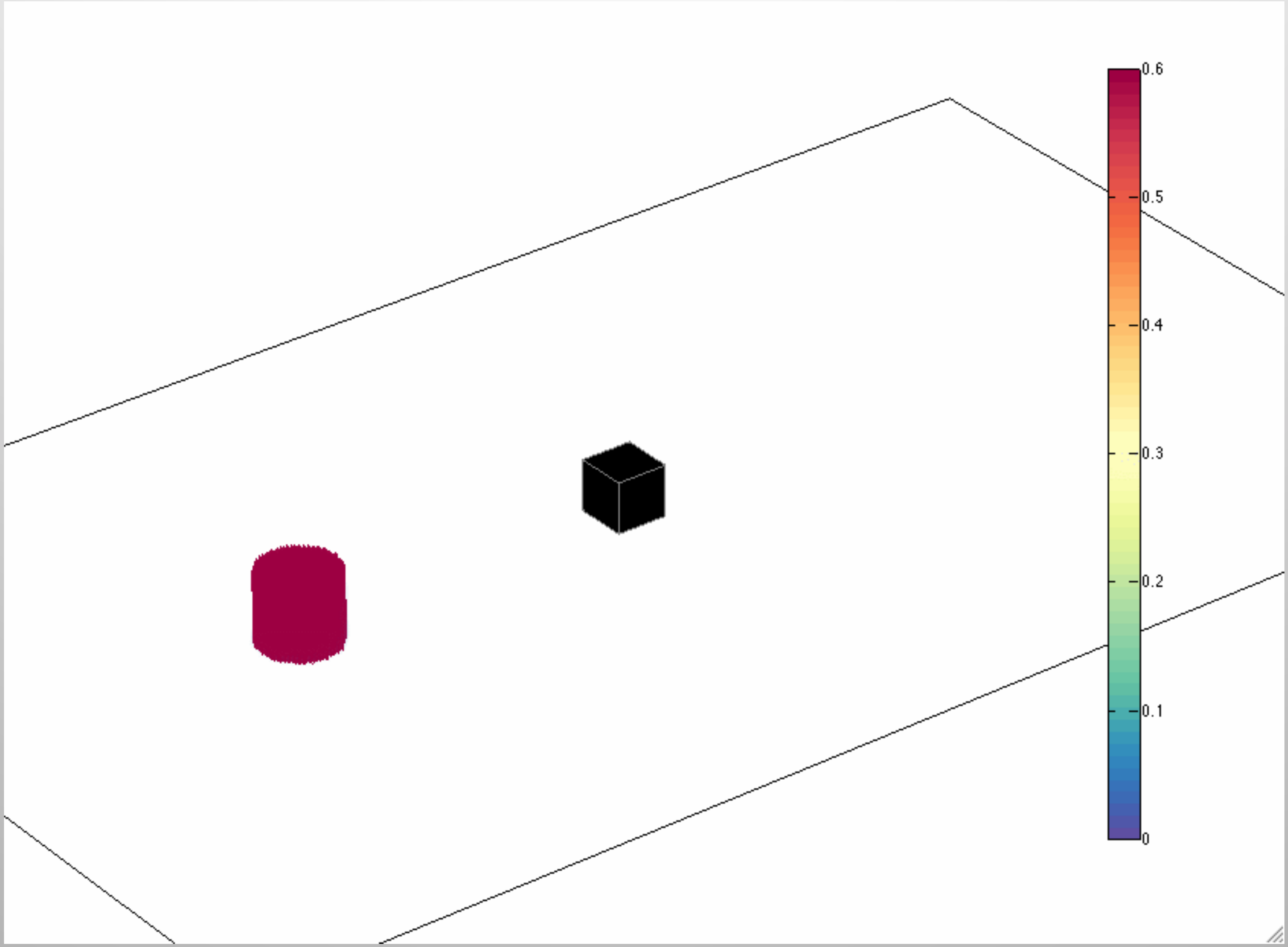


Deaves (1985)

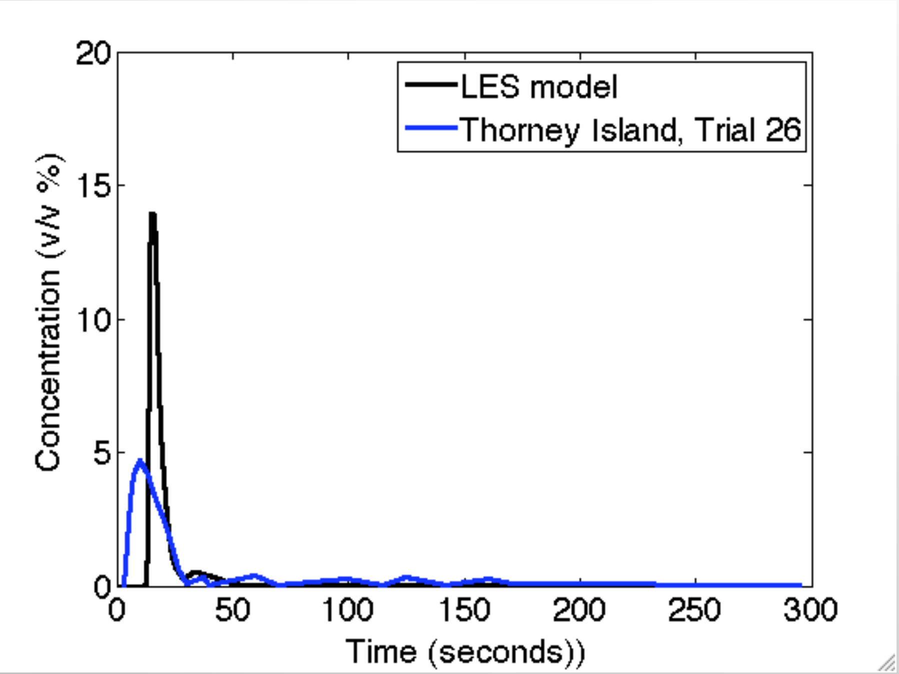


McQuaid and Roebuk (1985)

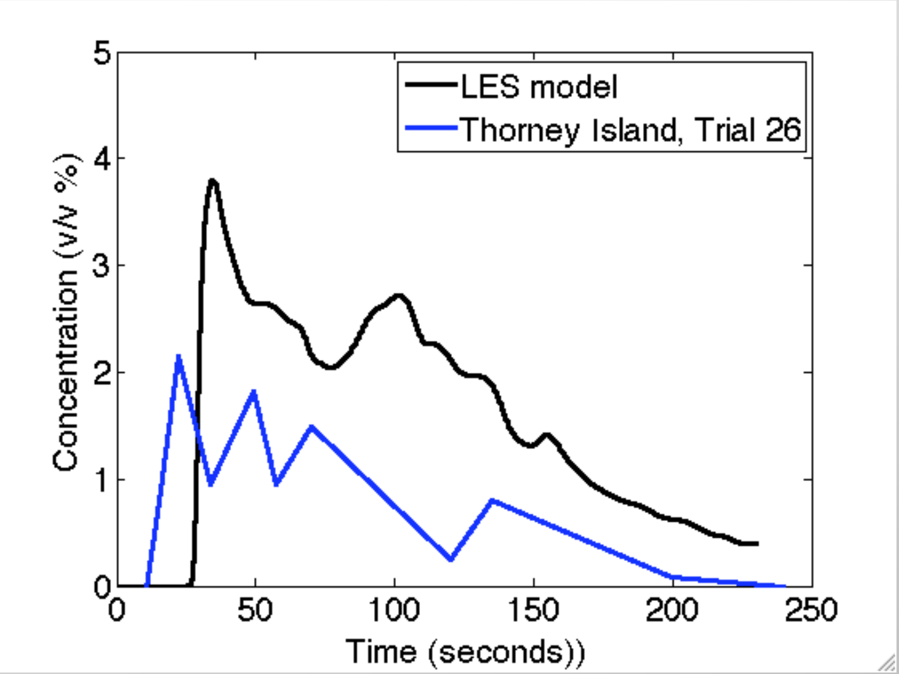
LES model



LES model validation



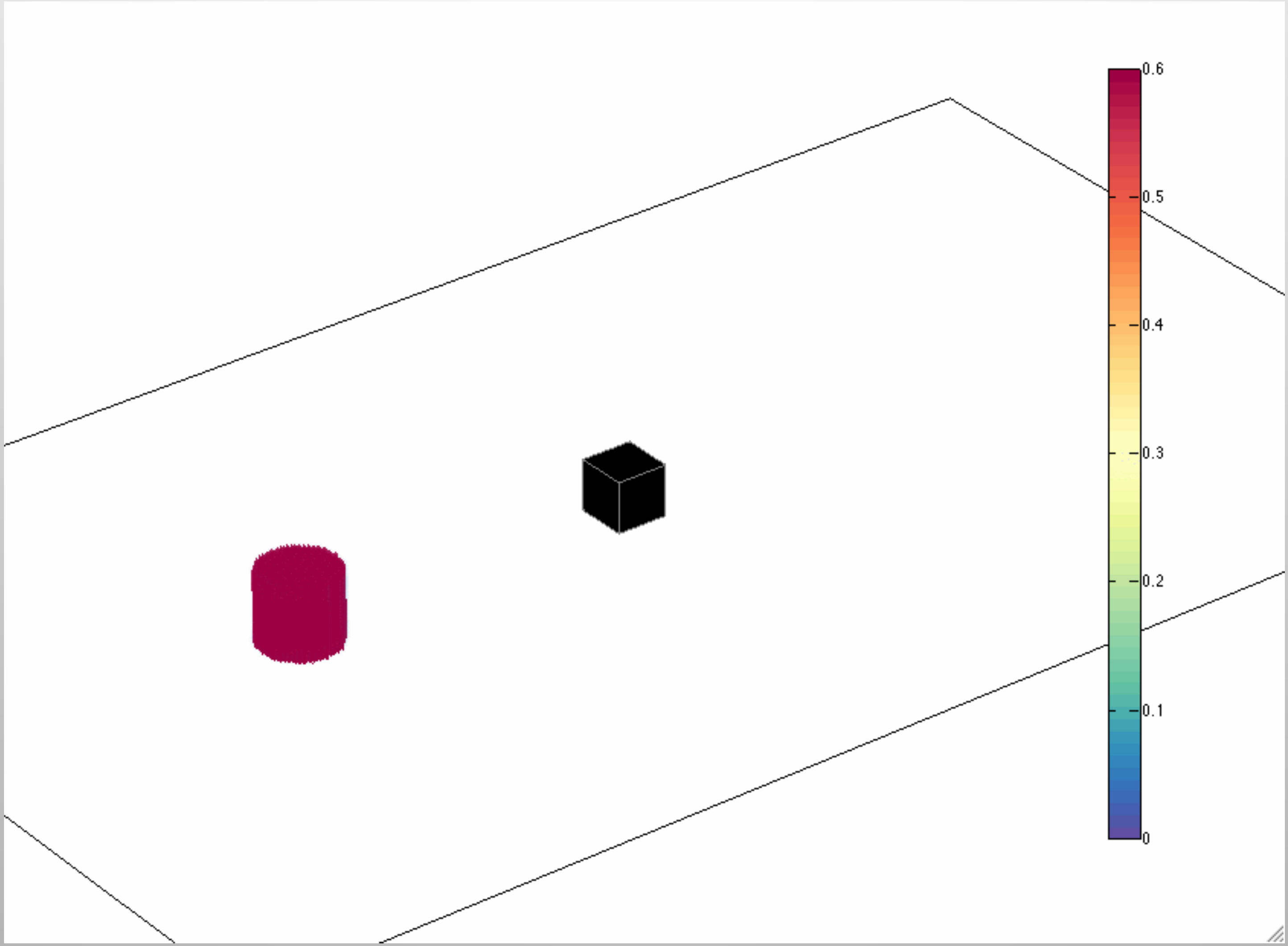
Windward face



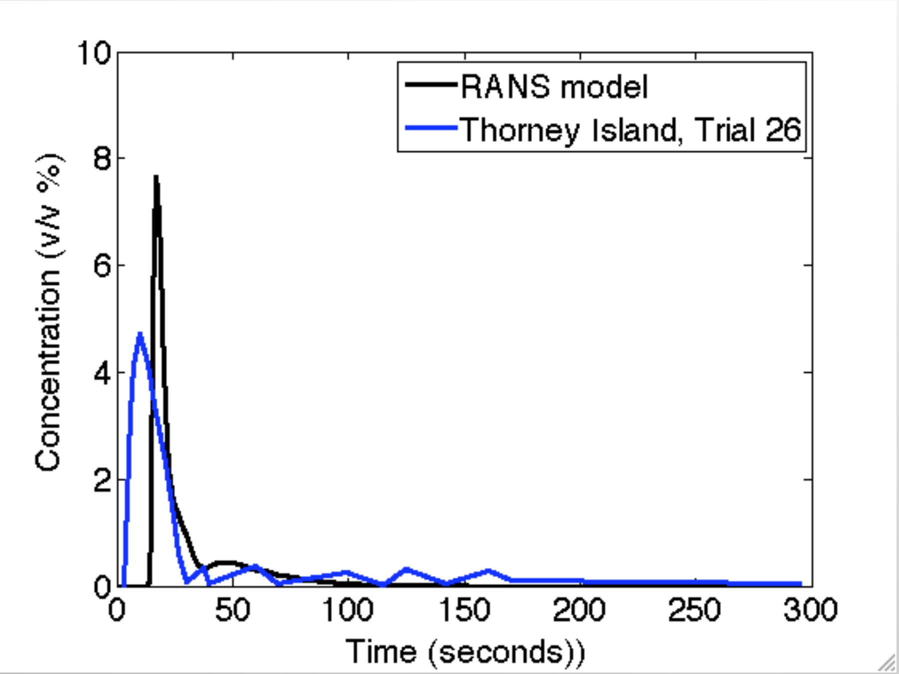
Leeward face

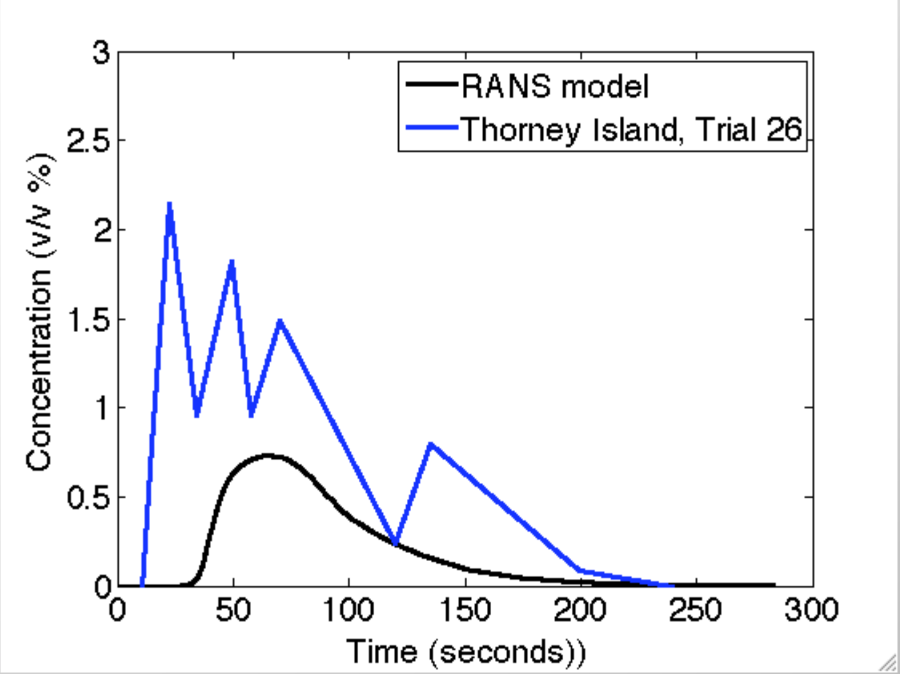
- Qualitative, the model produces similar looking dense gas cloud
- Higher peak concentrations are predicted by the model on both windward and leeward faces
- The arrival time of the cloud is well predicted by the model

RANS model



RANS model validation





Windward face

Leeward face

- Qualitative, the model produces similar looking dense gas cloud
- Higher peak concentration is predicted by the model on the windward face
- Lower peak concentration is predicted by the model on the Leeward face
- The arrival time of the cloud is well predicted by the model

Validation

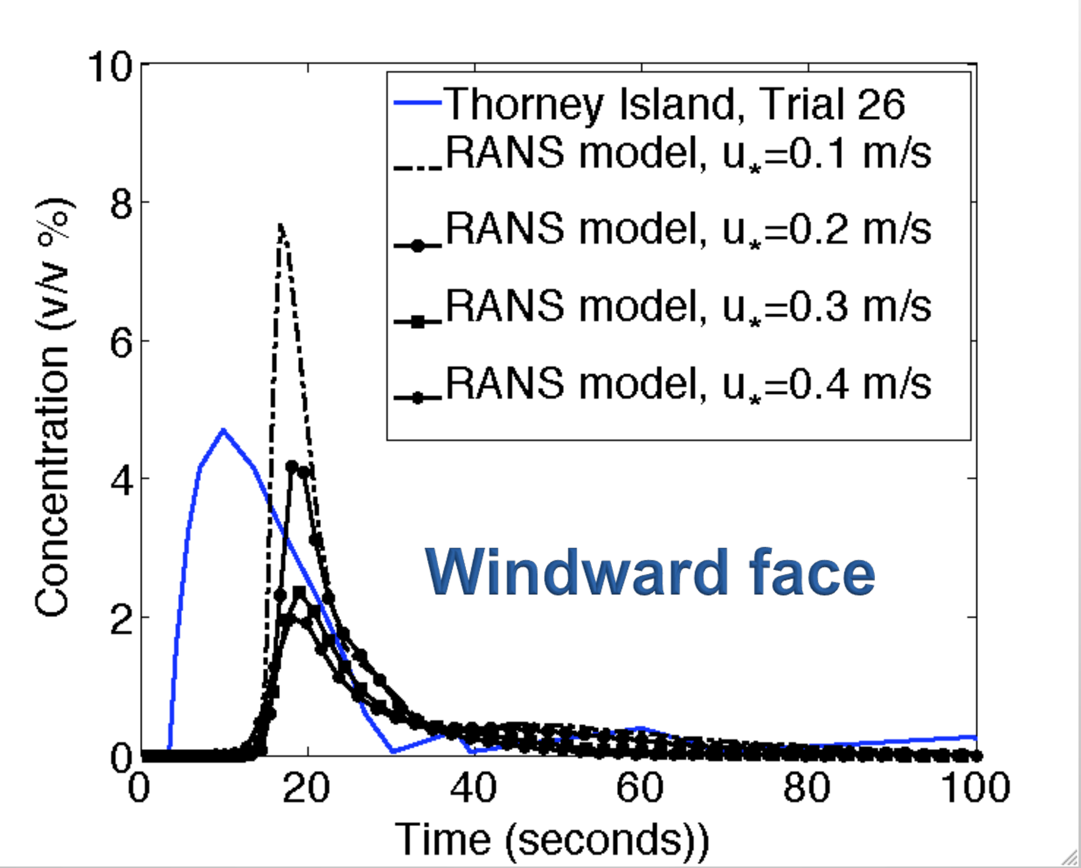
- To understand why models could not accurately predict the peak concentration correctly, we decided to study closely the effect of inflow turbulence
- RANS model was chosen as it was easy to vary the inflow turbulence by changing the the friction velocity
- The inflow velocity is specified by a log-law

$$u = \frac{u_*}{k} \ln\left(\frac{z}{z_o}\right)$$

$$v_T = (kz)^2 \left(\frac{du}{dz}\right) = kzu_*$$

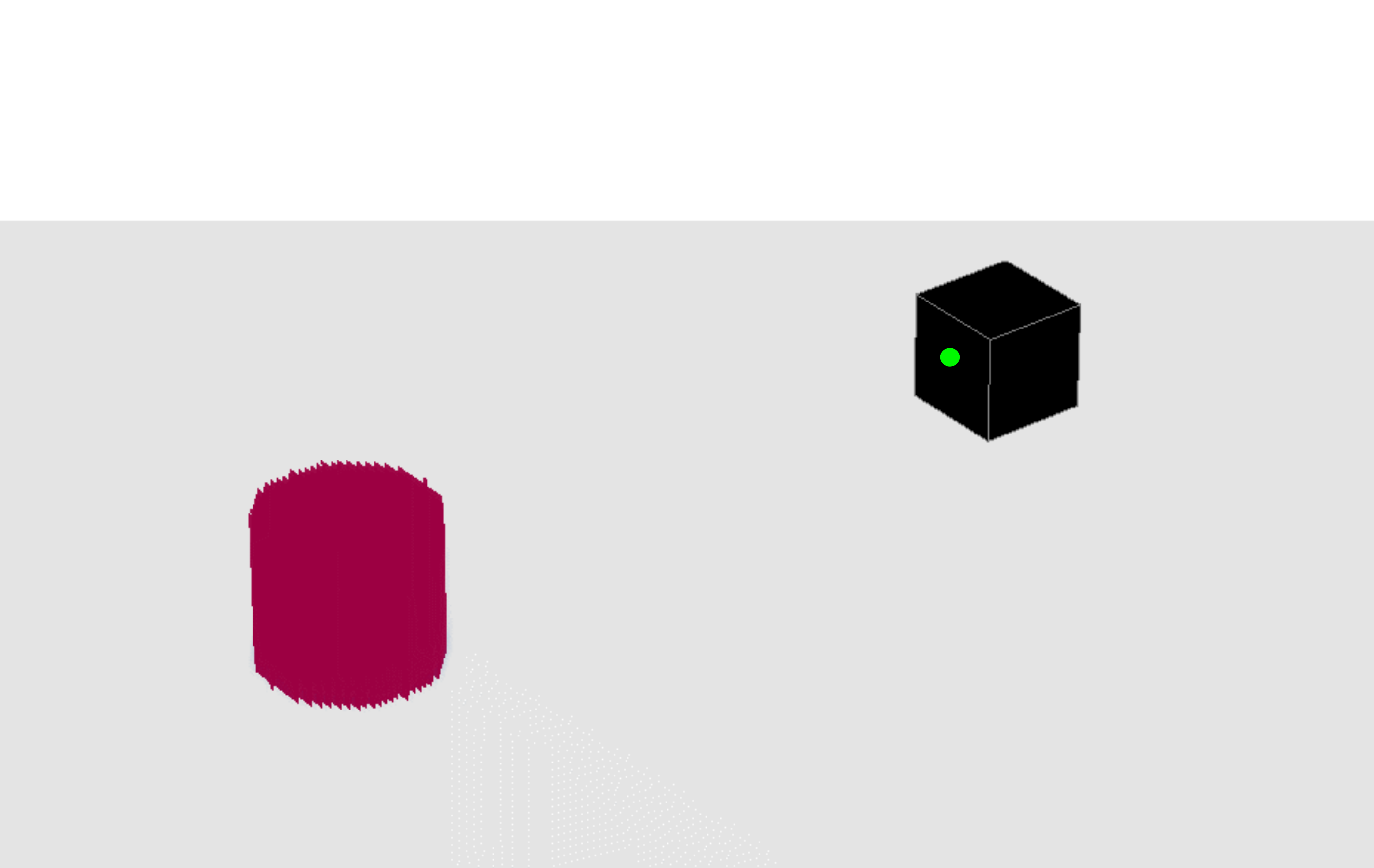
- Changing the friction velocity u_*, changes the inflow turbulence

RANS model validation



- **The peak concentration predicted by the model on the windward face is found to be very sensitive to the friction velocity**
- **Higher friction velocity produces a lower concentration value because of more mixing at the cloud top.**

RANS model validation



- The measurement was taken at 6.4 m on the front face of the cube.
- The location is very close to the top of the dense gas cloud and hence the concentration is very sensitive to the inflow turbulence

Conclusions

- Both the models are able to predict the concentration relatively well.
- LES produced dense gas clouds looks more realistic
- Friction velocity has a significant effect on the concentration value
- Both the models have similar computational cost for dense gas dispersion simulation