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Atmospheric Flow Validation for Contaminant Transport

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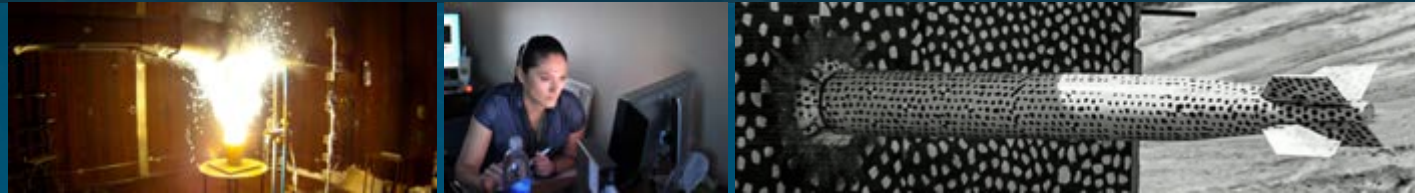
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Atmospheric Flow Validation for Contaminant Transport



PRESENTED BY

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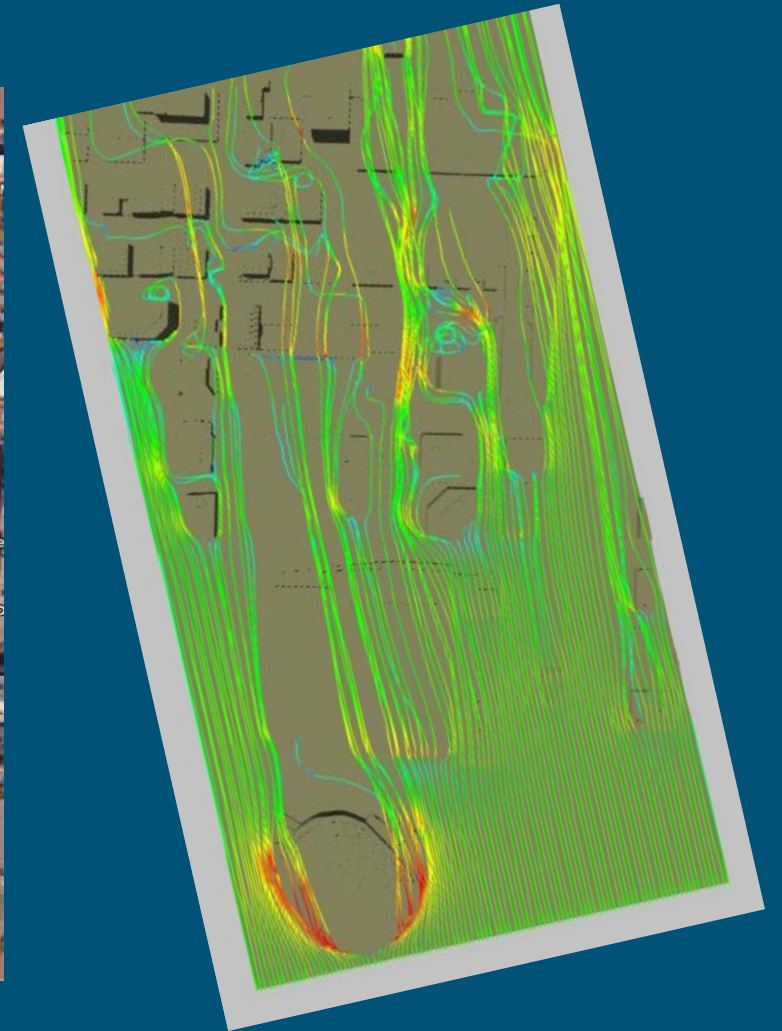
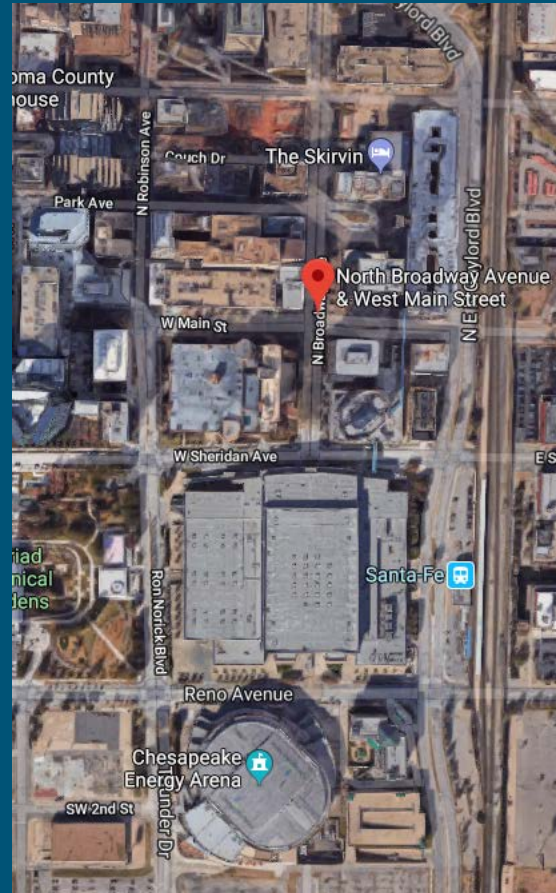
ASME Verification and Validation Symposium, Las Vegas, NV,
May 15-17, 2019

Atmospheric flow with contaminant transport is a challenging simulation problem

2



- Large length scales required
- Complex geometry with separated flow
- Little/sparse validation data available

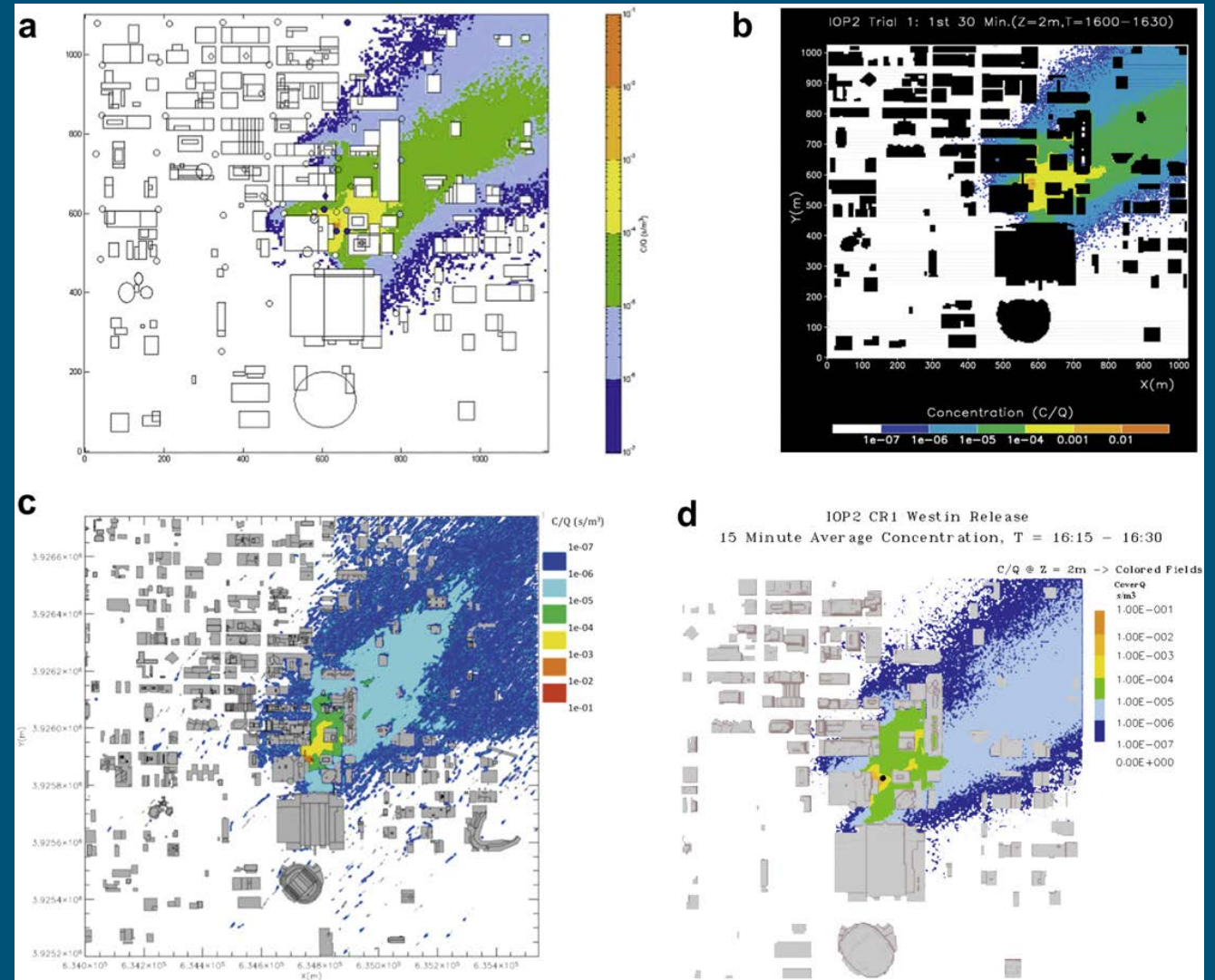


Oklahoma City Downtown Area – Result on right rotated for geometric alignment

Many dispersion approximation models have been used previously



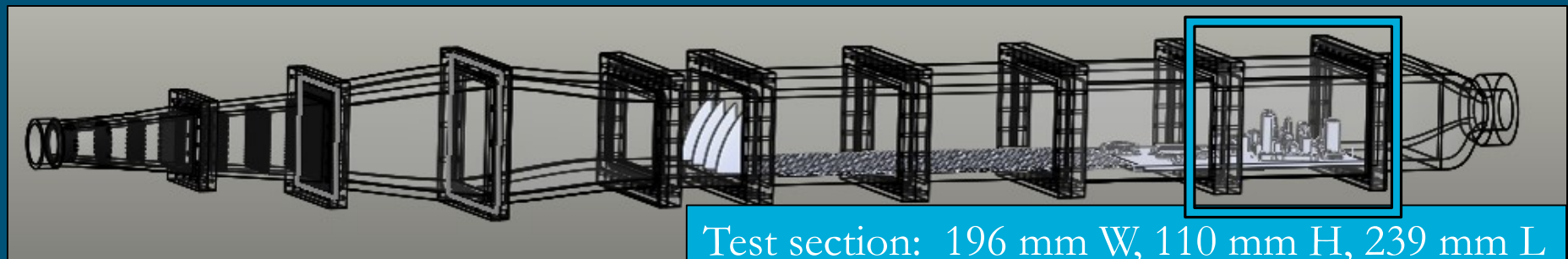
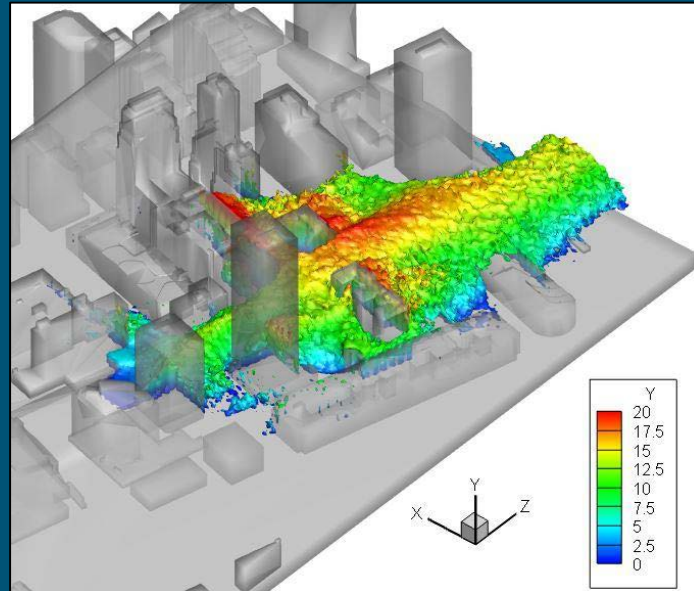
- a – QUIC by Los Alamos National Laboratory
- b – 3DWF by Army Research Laboratory
- c – Urban Lagrangian Model by Israel Institute for Biological Research
- d – MSS by Aria Technologies and SAIC
- Computational Fluid Dynamics (CFD) has higher fidelity and is likely to be more accurate



Hanna2011 - Comparisons of JU2003 observations with four diagnostic urban wind flow and Lagrangian particle dispersion models

4 Scaled validation data were measured in a medical MRI machine

- Experiments conducted at Stanford
- Methods
 - Magnetic Resonance Velocimetry
 - Magnetic Resonance Concentration
- CuSO_4 tracer in water
- Full 3D data, $\text{Re}_{D_H} = 36,000$
- Time-averaged over 60-90 minutes
- 0.8 mm resolution, 13.4 million voxels
- $U_{\text{velocity}} = 4\%$ of measured value
- $U_{\text{concentration}} = 5.5\%$ of measured value
- $U_{\text{space}} = 0.4 \text{ mm}$ (1/2 voxel)

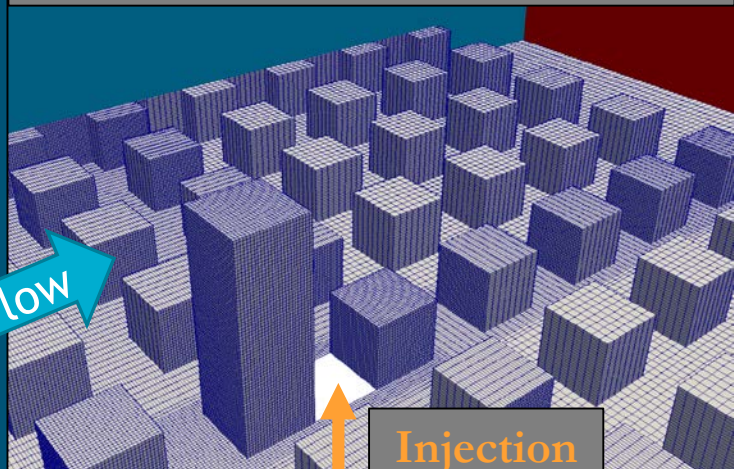


Test section: 196 mm W, 110 mm H, 239 mm L

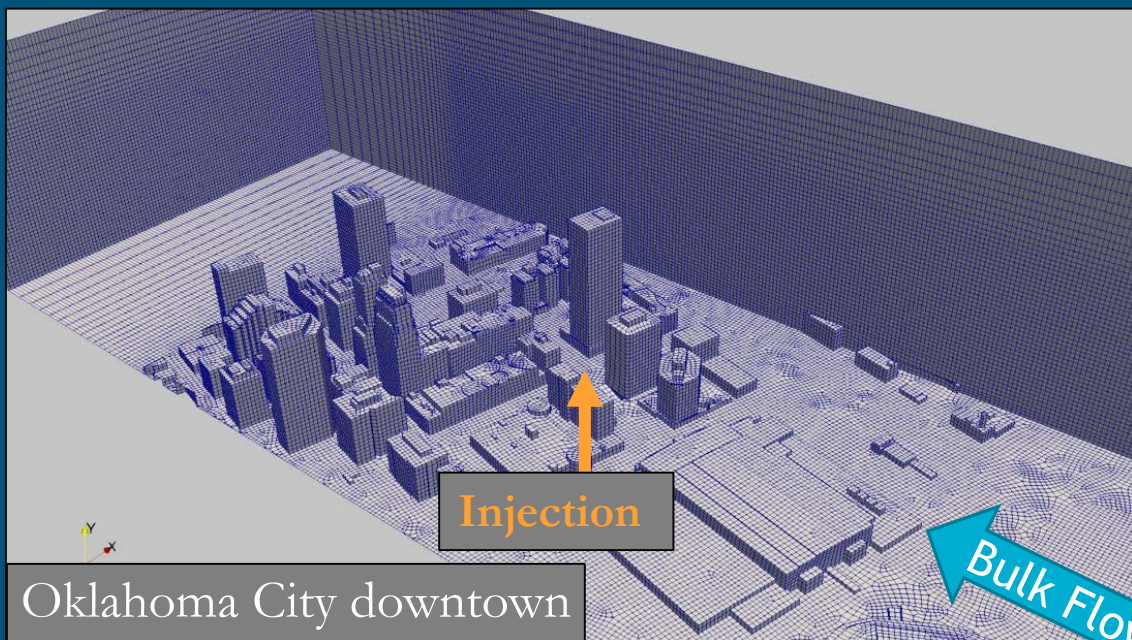
This program has investigated three urban geometries



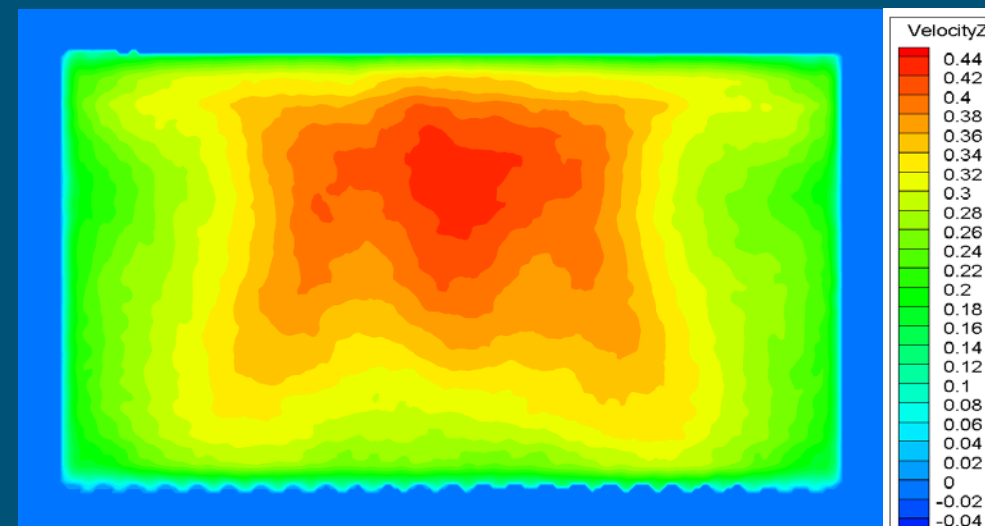
Gridded building array at 90°



Gridded building array at 45°



Oklahoma City downtown

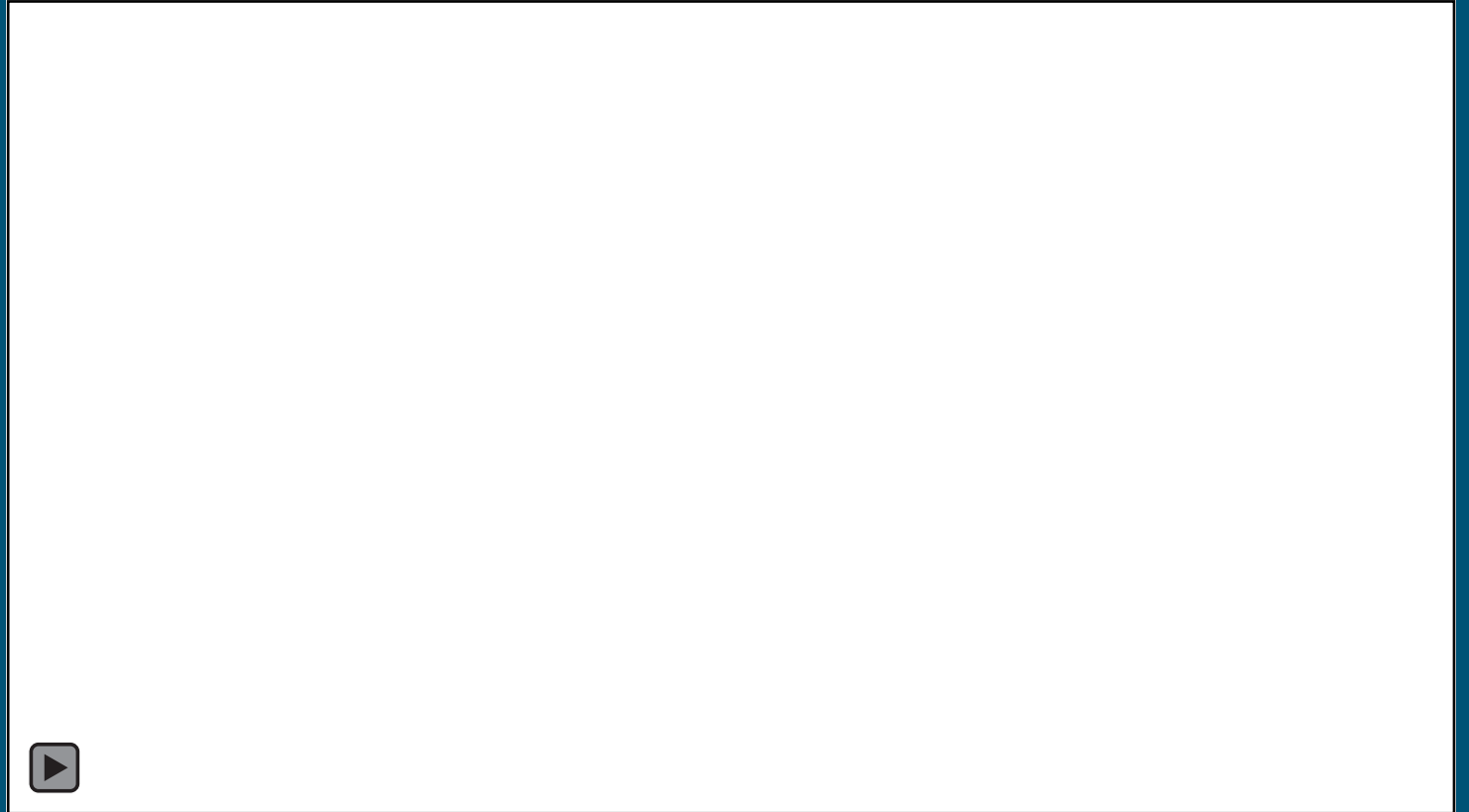


Measured inflow example

Three models were used and compared



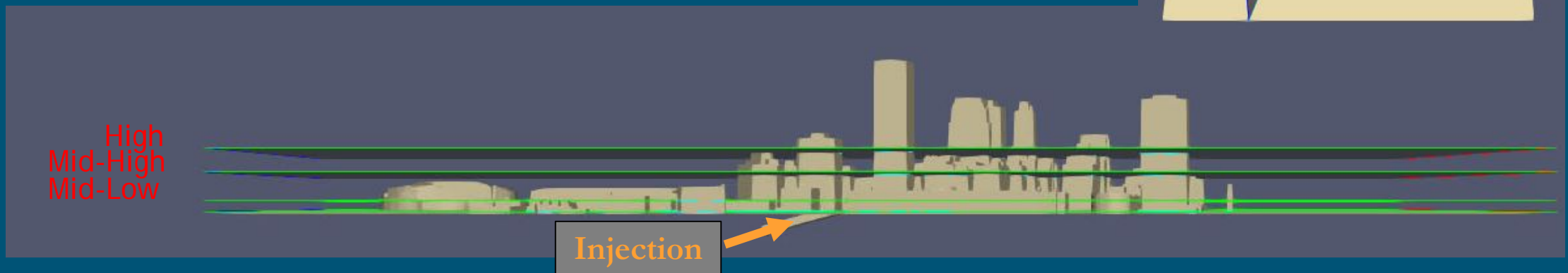
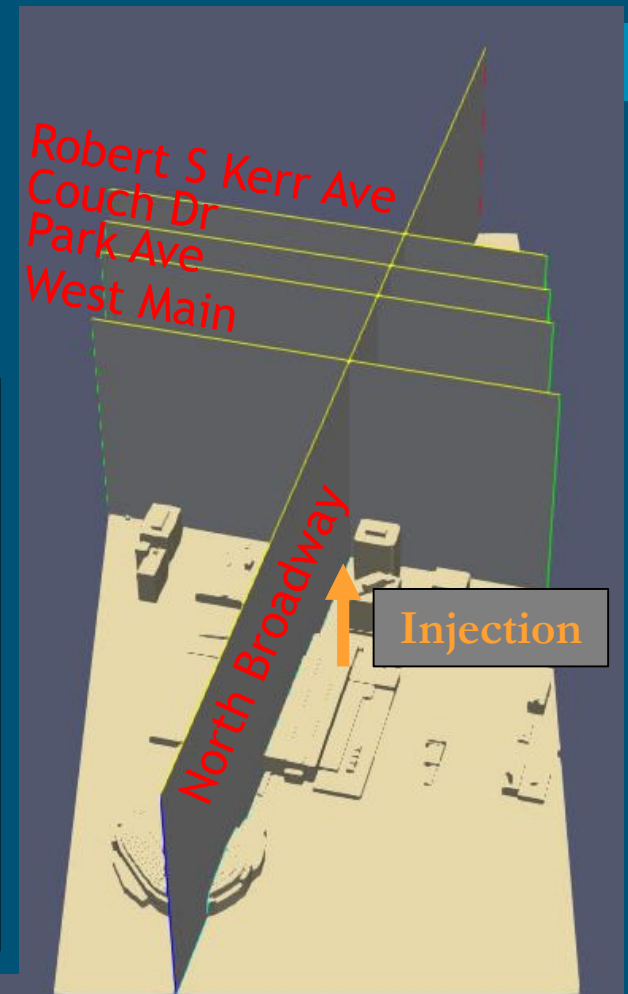
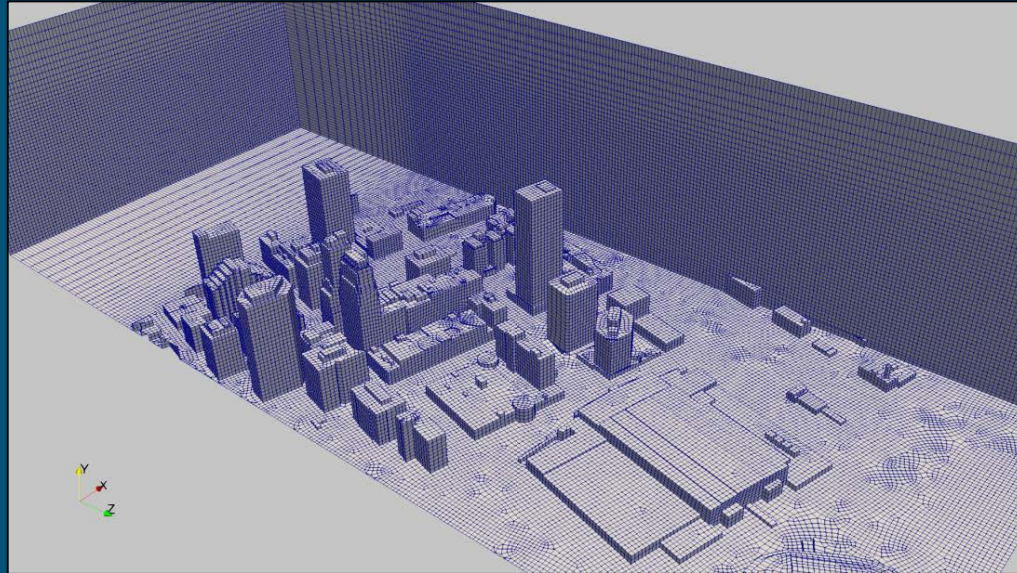
- Large Eddy Simulation (LES)
subgrid scale kinetic energy
(KSGS) (Kim and Menon, 1997)
- Time-filtered Navier-Stokes
(TFNS)
- $k - \epsilon$ RANS model



LES prediction for 90° case shows large separation area downstream
of tall building

This work details the Oklahoma City case

- Real urban environment
- Reliable validation data
- Best practices on grid refinement setup
- 1:2500 scale

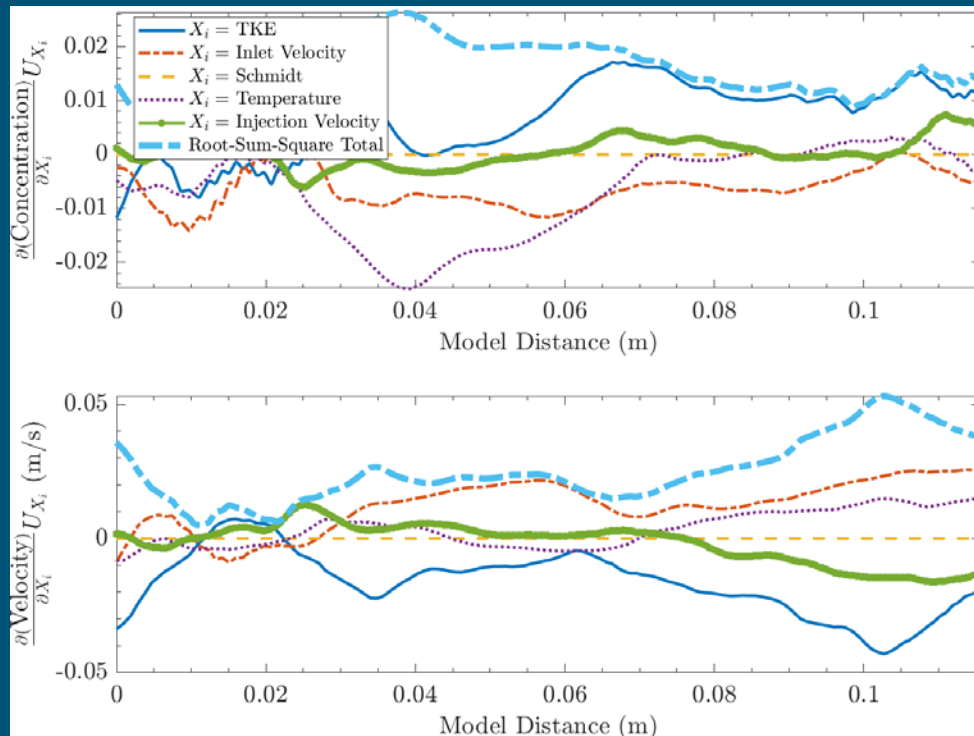


A parameter study was performed with five parameters

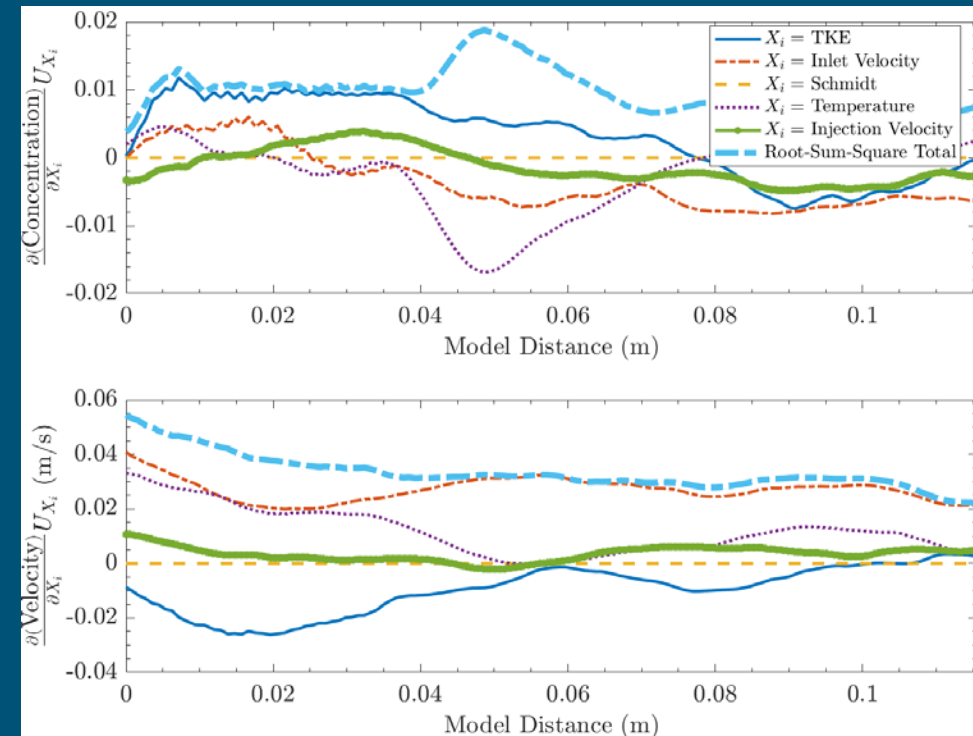


Parameter	Baseline	Variation
Turbulent kinetic energy	0%	+10%
Inlet velocity	Measured	±5%
Schmidt number	0.9	±0.2
Temperature	21°C	±25%
Injection velocity	22.5 cm/s	±10%

- Concentration was sensitive to TKE
- Velocity was most sensitive to inlet velocity



North Broadway-Medium Low



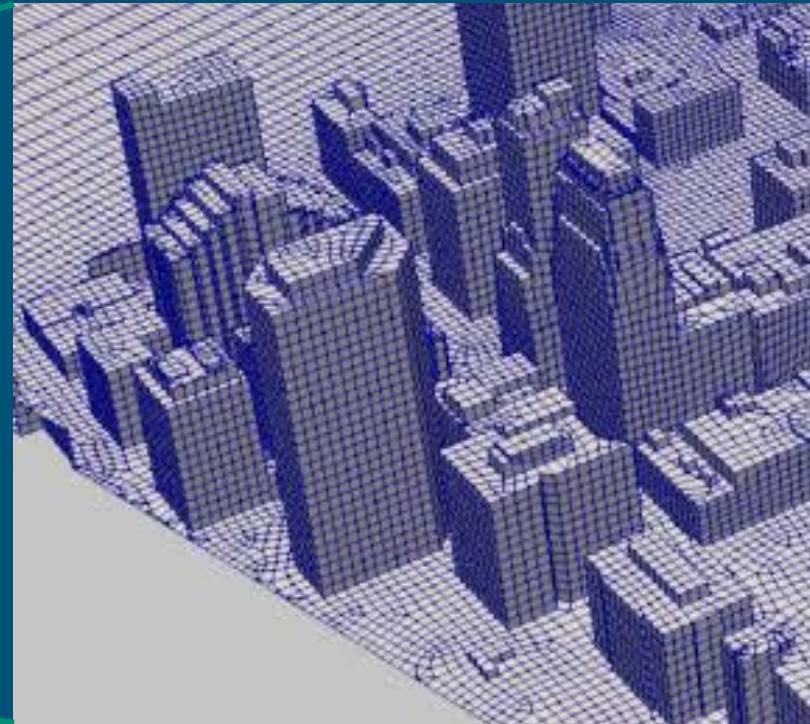
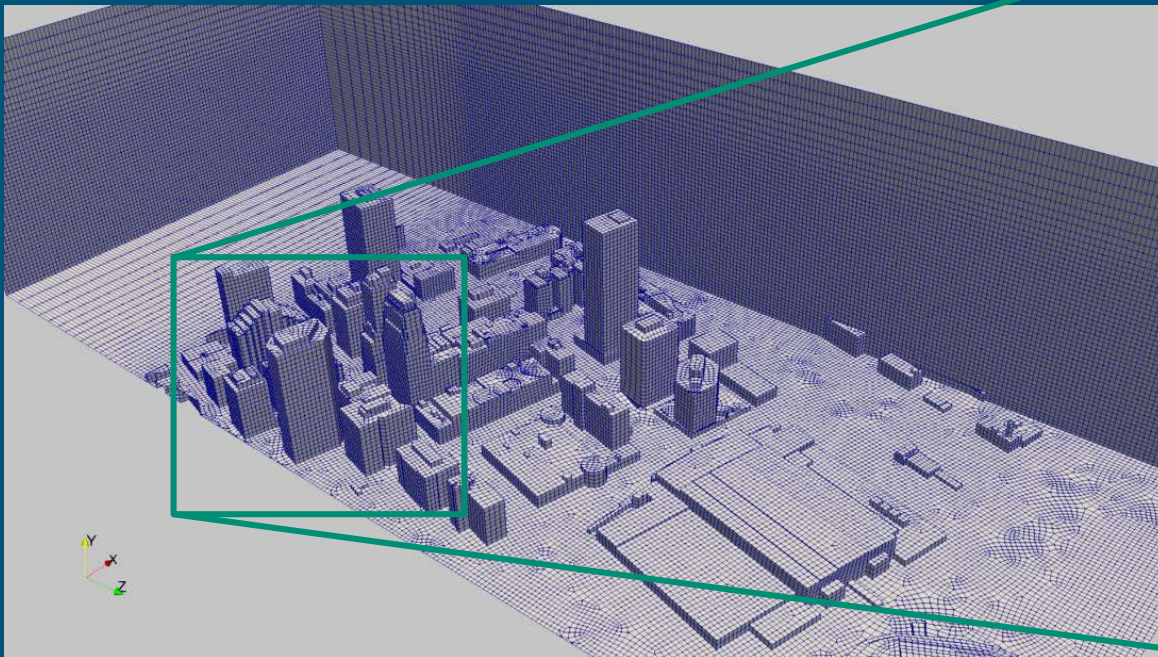
North Broadway-Medium High

Grid refinement was systematic with Hexagonal elements



Experimental resolution is 0.8 mm

Mesh	Hex Typical Size	Nodes
Coarse	1.7 mm	1.5M
Medium	0.85 mm	12M
fine	0.57 mm	41M

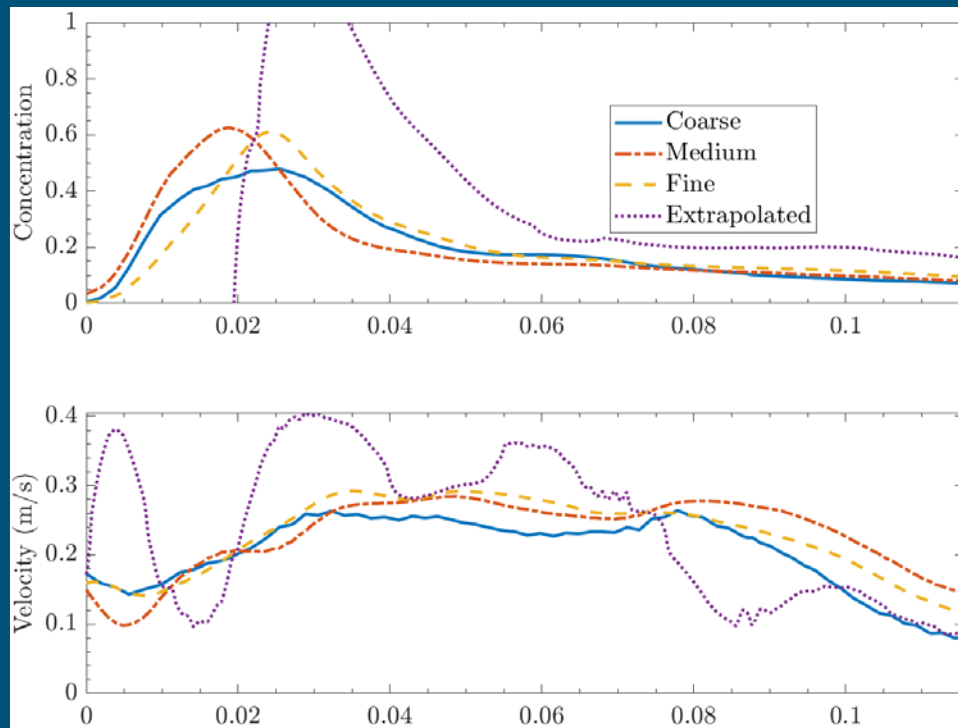


Full Hexahedral Mesh

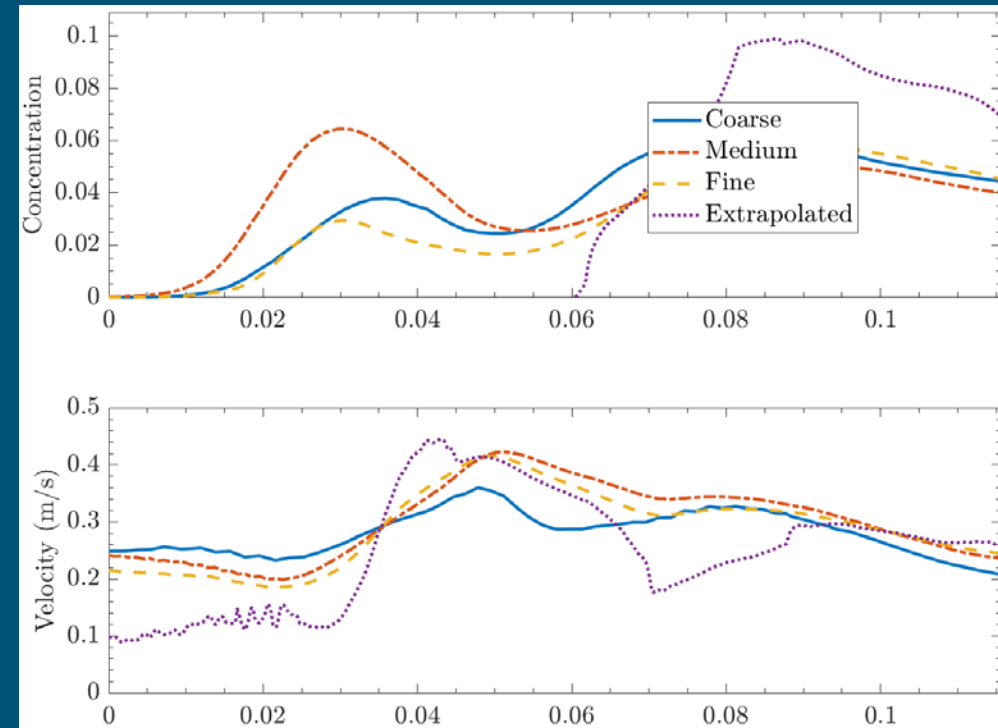
Grid convergence issues for LES



- Because the level of eddy resolution changes with mesh refinement, the results are a compound of mesh resolution and the changing eddy resolution scale
- Richardson Extrapolation and uncertainty quantification using V&V-20 methods need adaptation
- Best practices need to be developed (perhaps maintaining filter length scale as in Bunge2005)



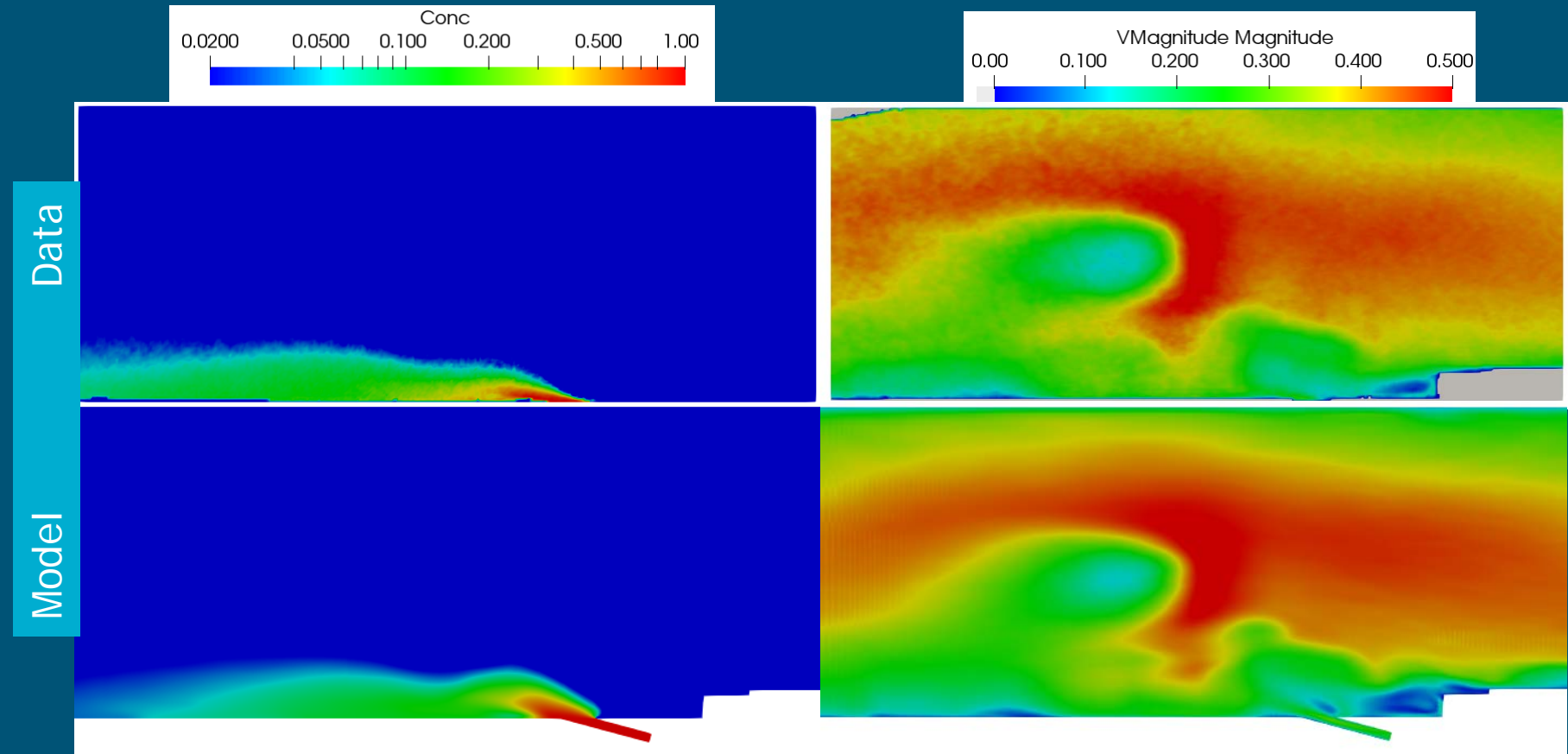
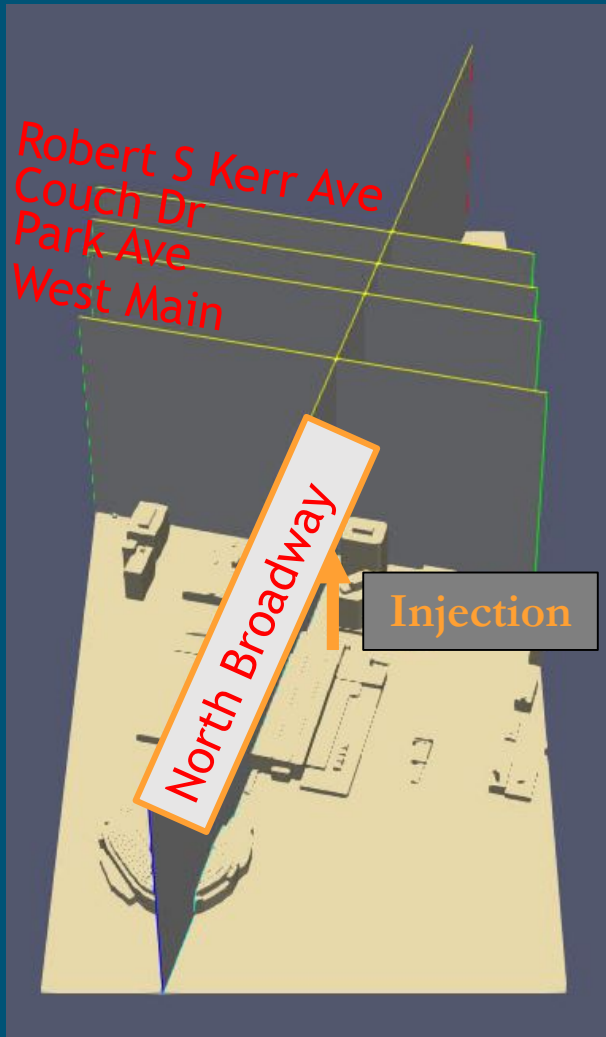
North Broadway-Medium Low



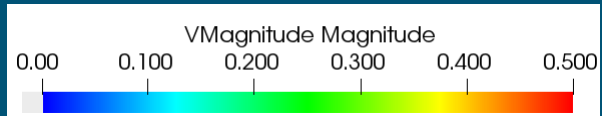
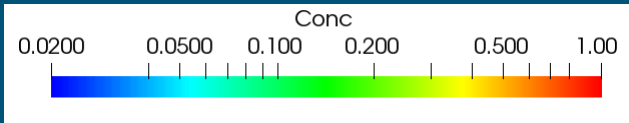
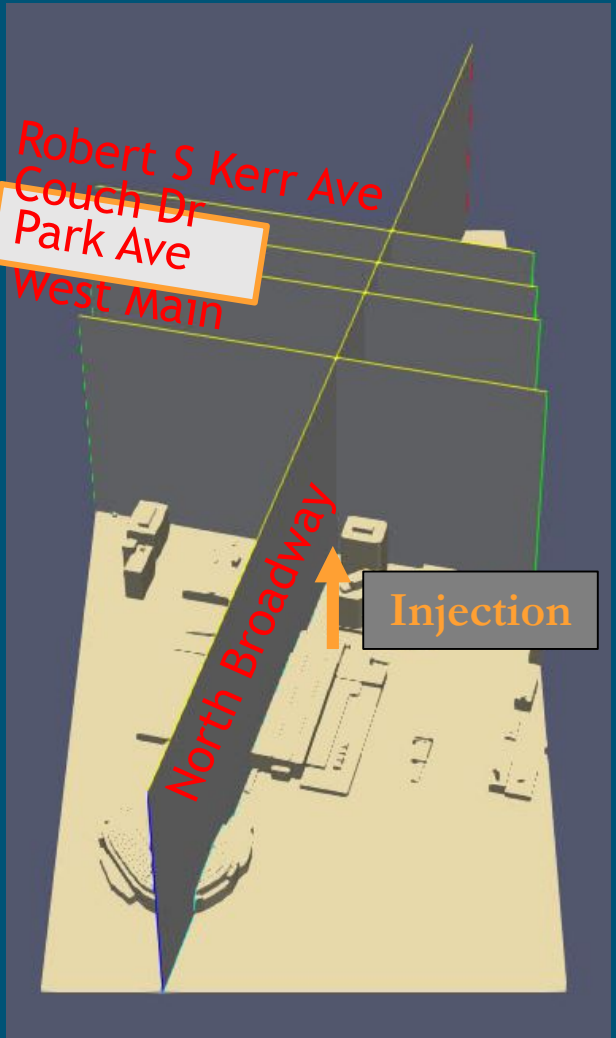
North Broadway-Medium High

Baseline simulation results

- LES, Medium mesh, hexagonal elements

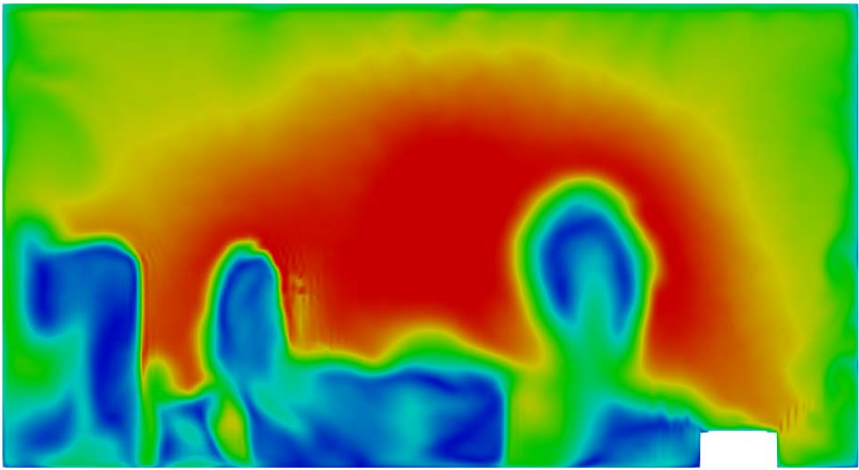
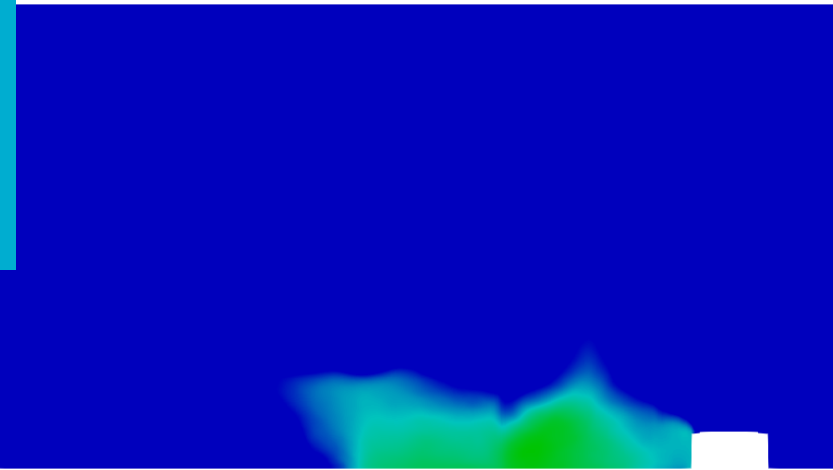
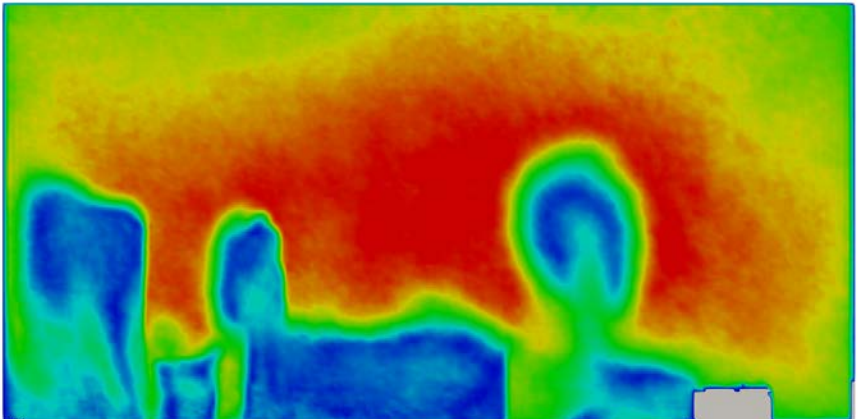
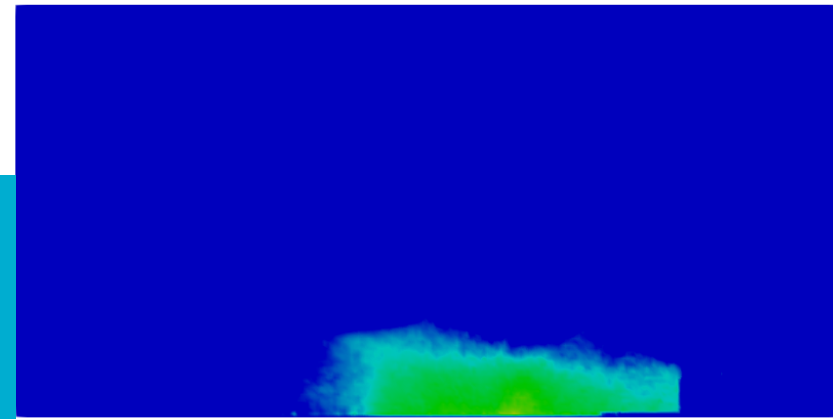


Viewgraph norm comparisons

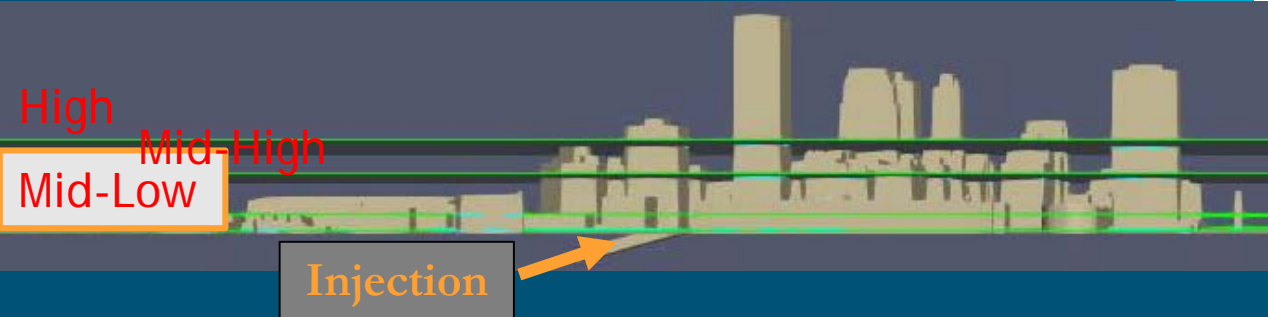
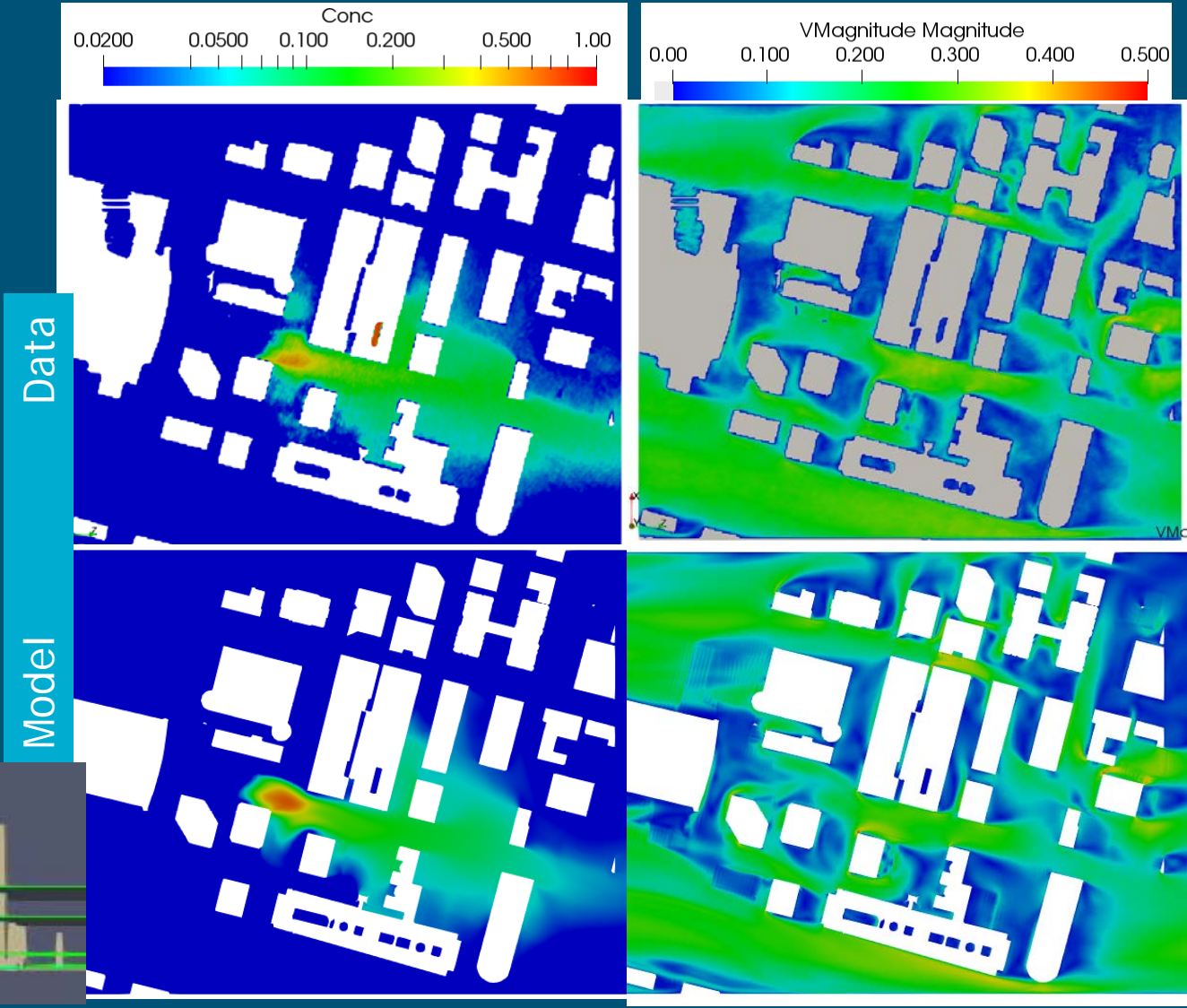


Data

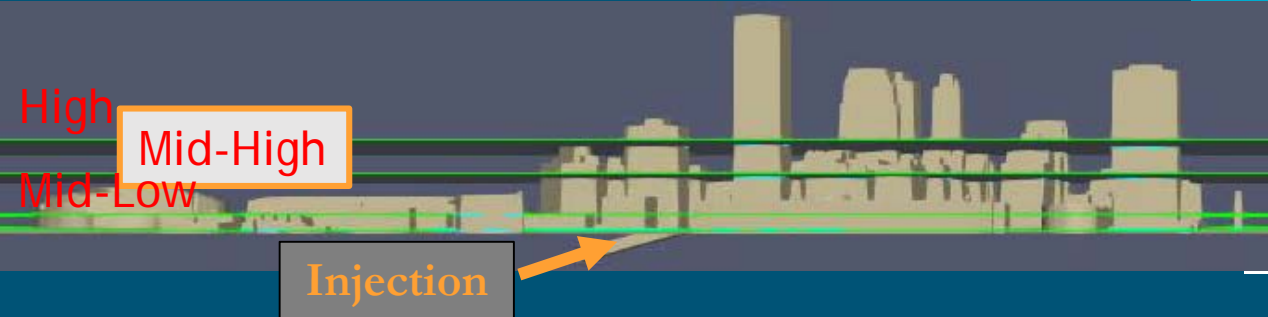
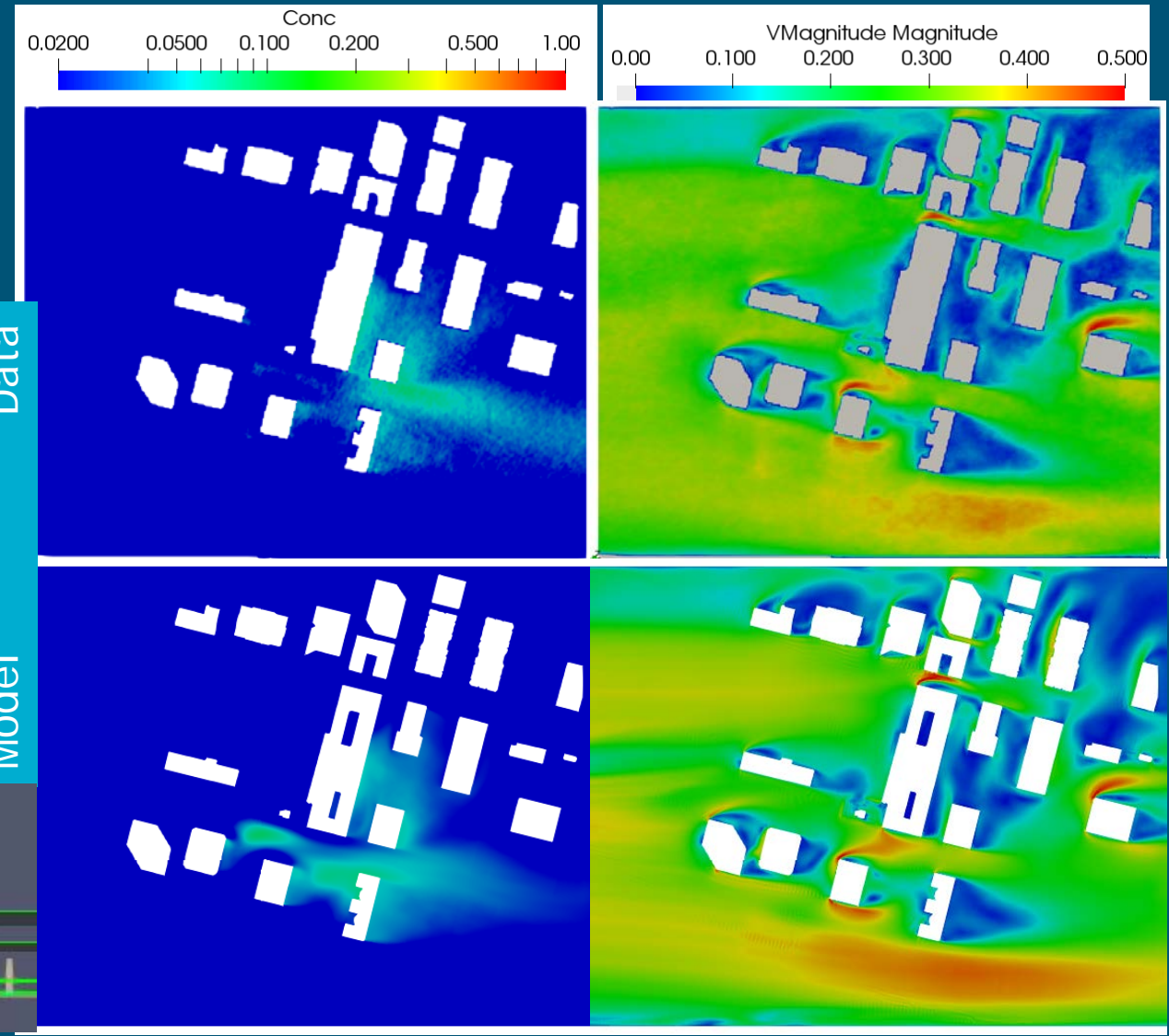
Model



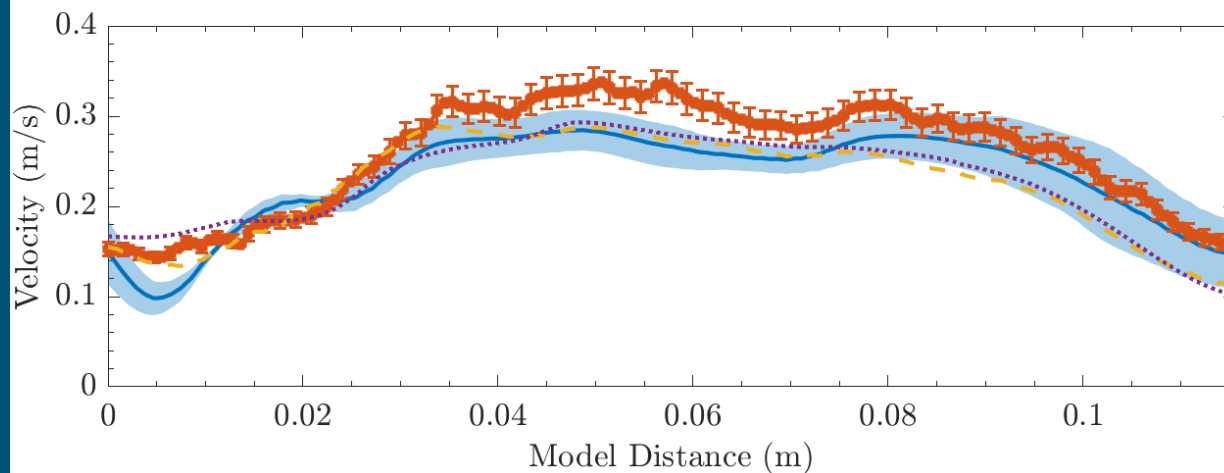
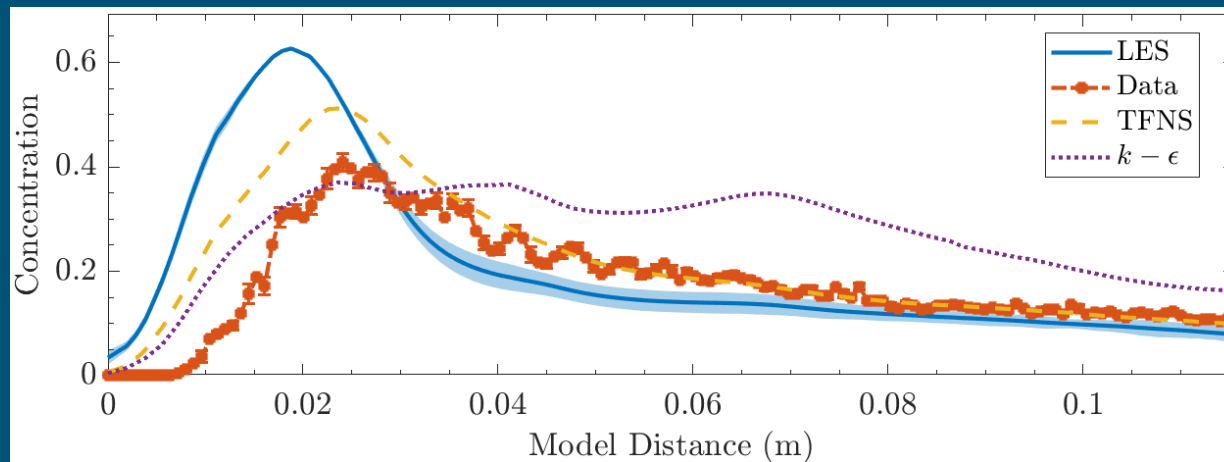
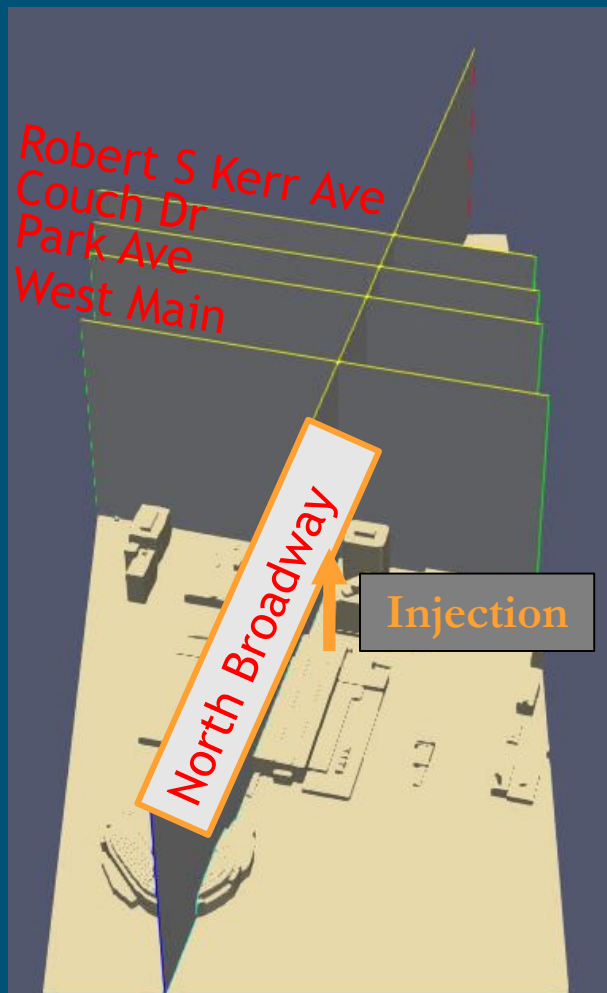
Viewgraph norm comparisons



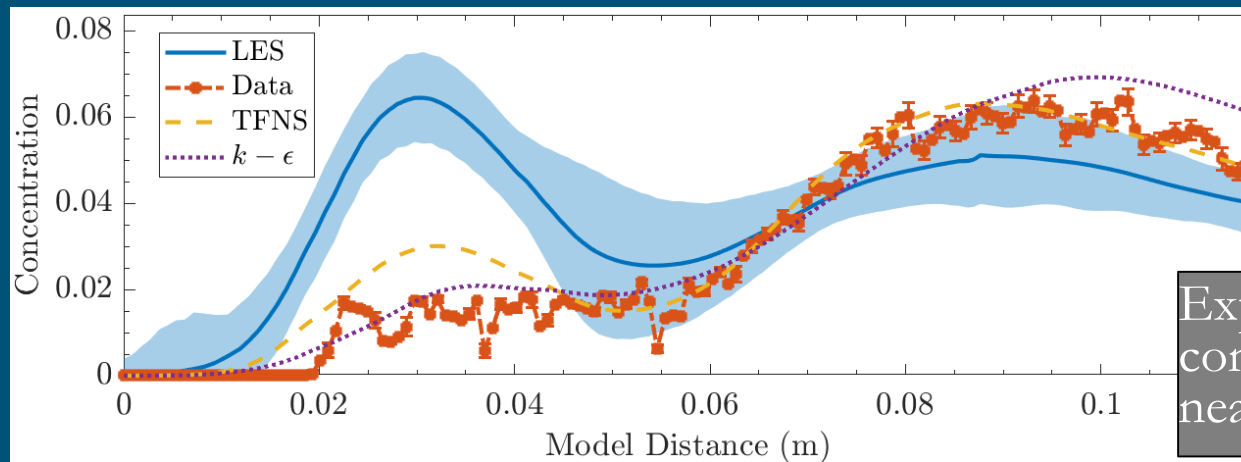
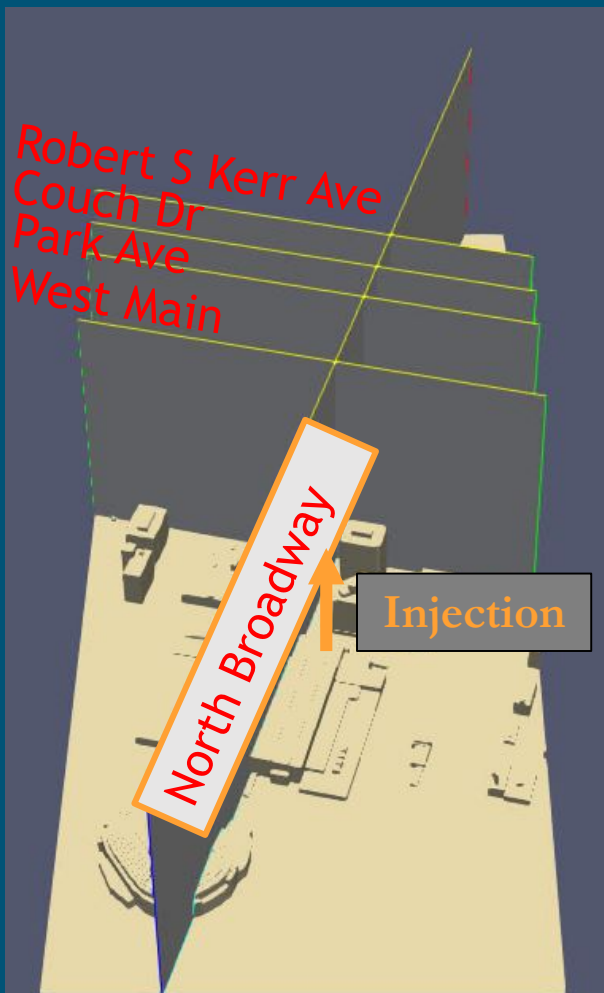
Viewgraph norm comparisons



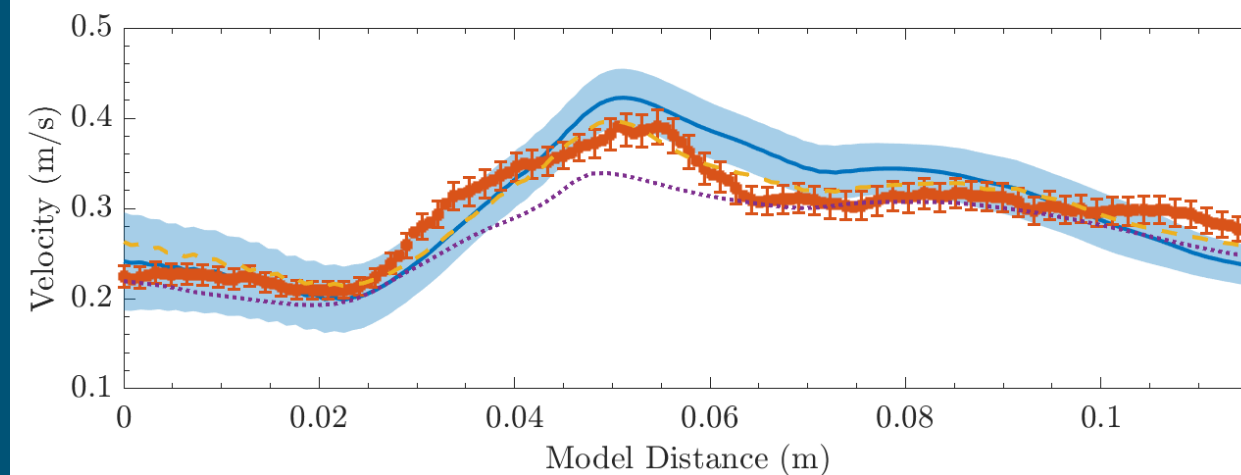
Line plots provide a detailed comparison



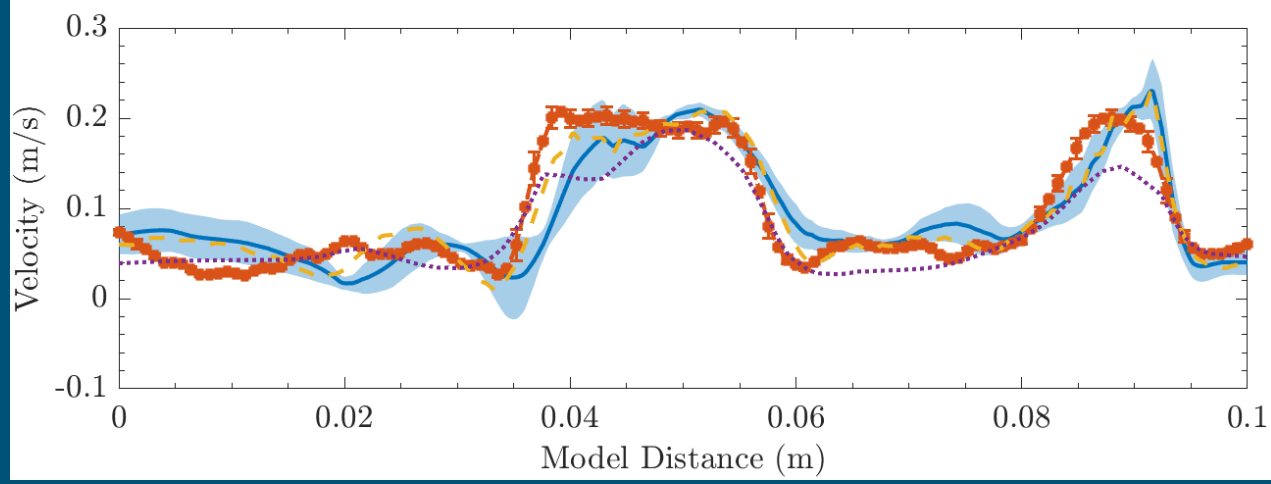
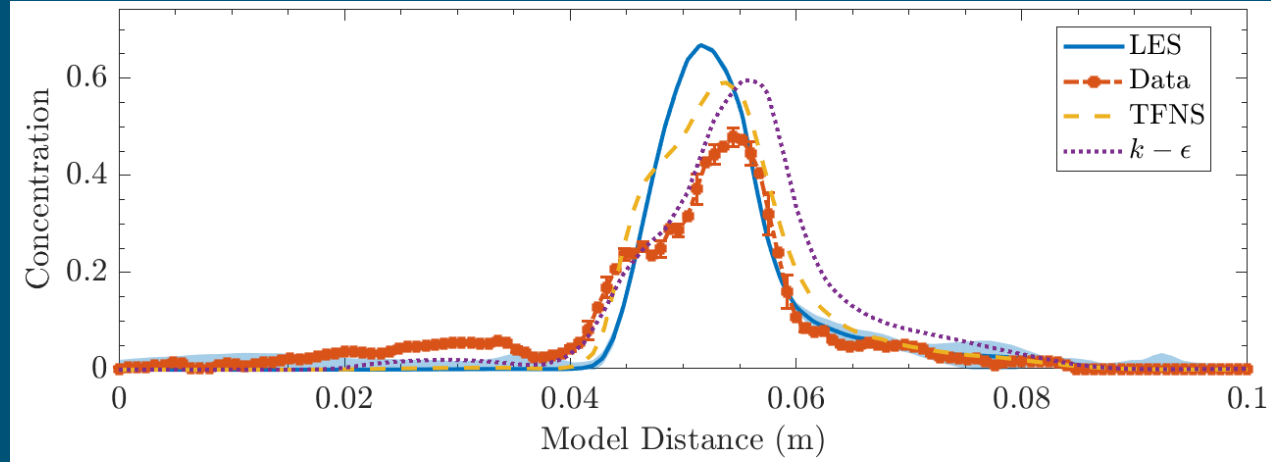
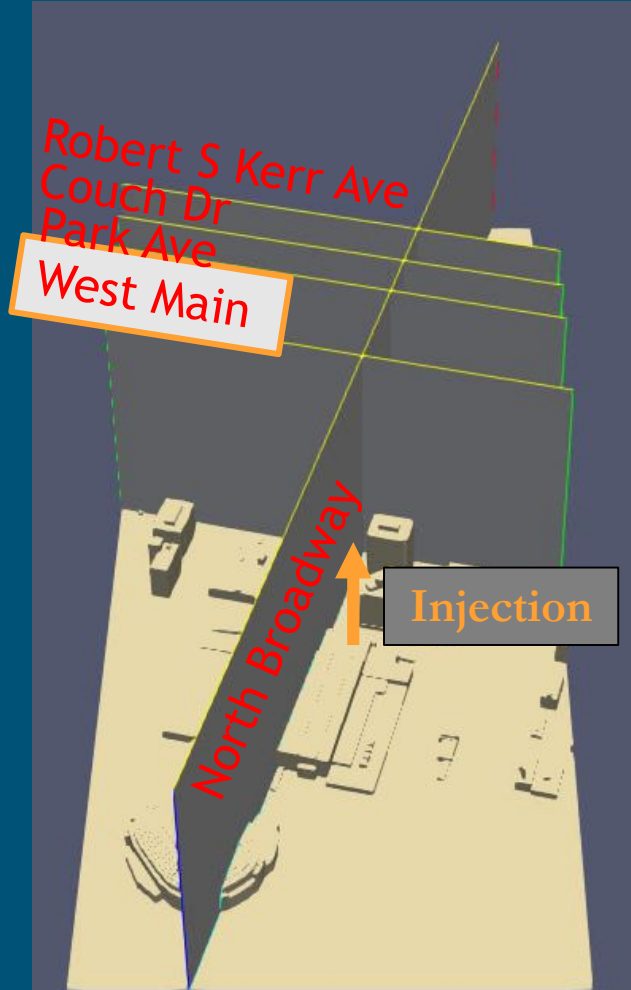
Line plots provide a detailed comparison



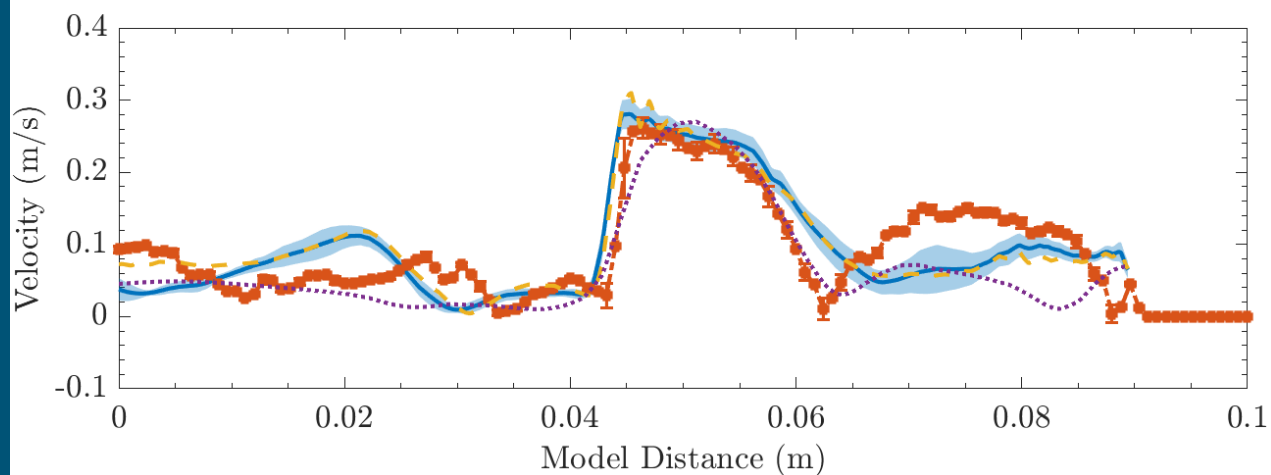
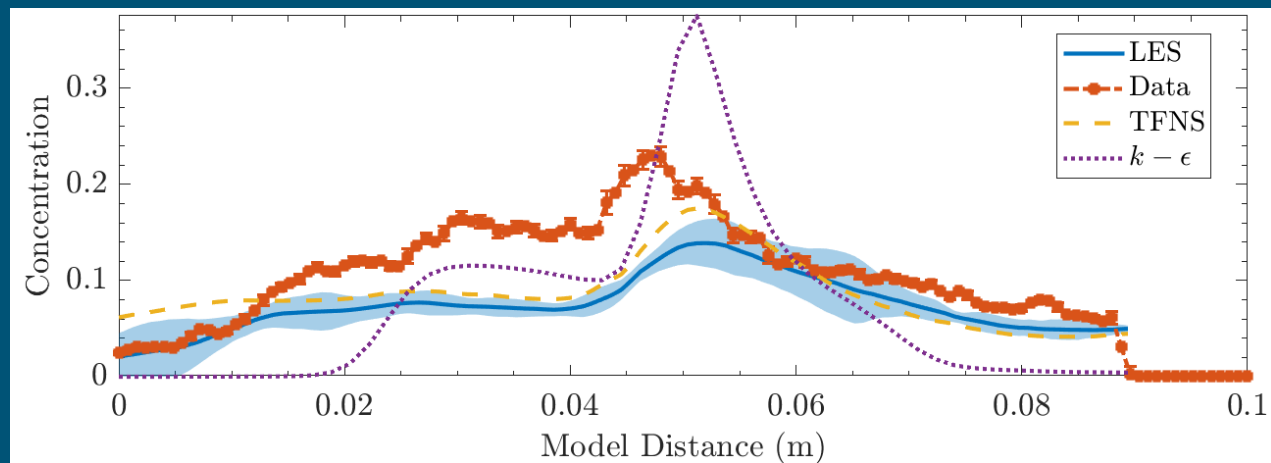
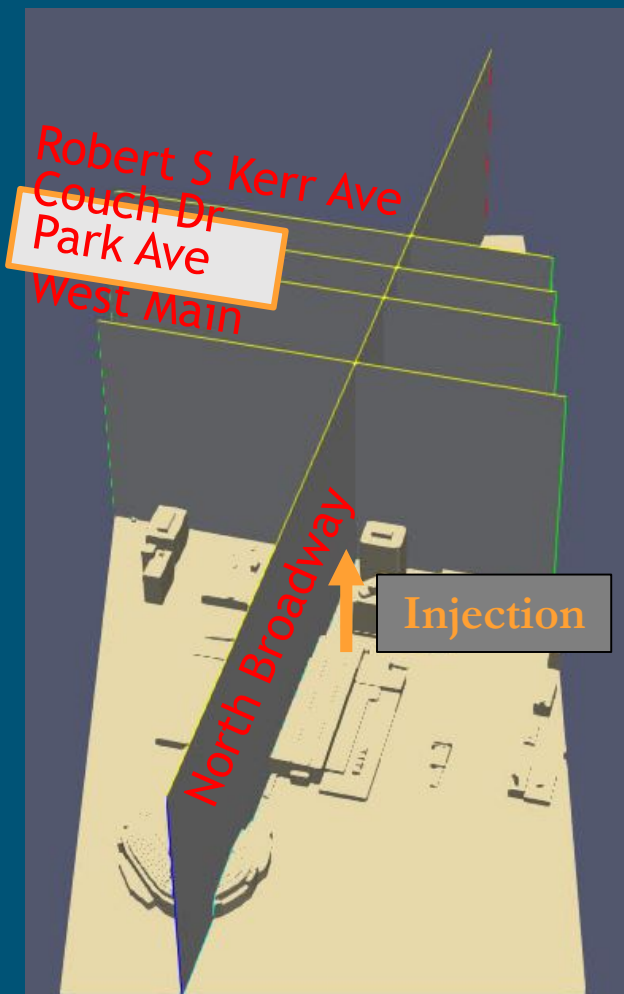
Experimental concentrations are near noise floor



Line plots provide a detailed comparison

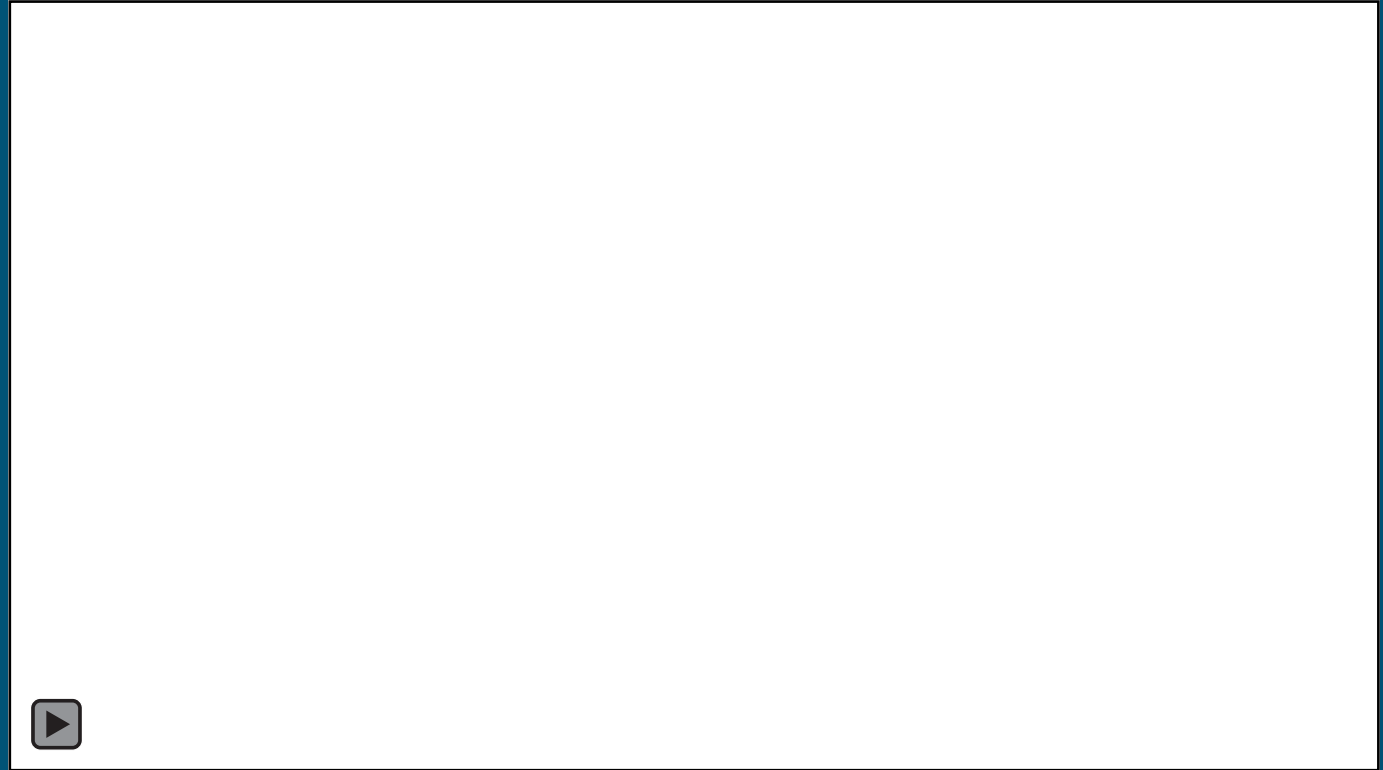


Line plots provide a detailed comparison





- The MRV and MRC techniques provide excellent coverage for validation data
- The simulations appear to have good accuracy (application-specific metrics should be evaluated)
- Future Work
 - Best practices for grid converge studies for LES should be developed
 - Terrain geometry



Purple is a 1% concentration