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Computational Comparisons to the Multi-stack MRC/MRV Dispersion Dataset

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Introduction

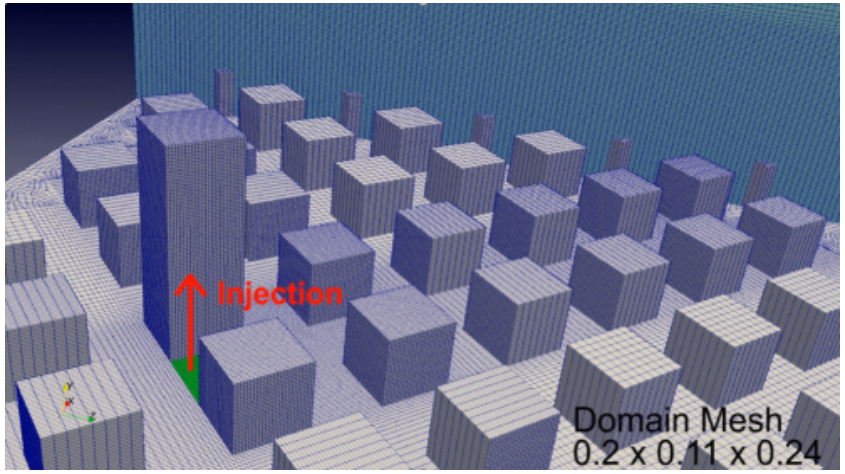
- MRC and MRV provide 3D data (velocity and concentration) for turbulent water flows in scaled urban geometries
  - Excellent validation data because inflow boundary is characterized
  - Geometric accuracy is high
- Additive manufacturing permits tests of geometries identical to models to manufacturing tolerance
- We have previously evaluated scenarios with single release points
  - This work evaluates a multi-stack scenario that includes plume mixing and interactions
- Methods for validating models are still a topic of

These aspects to this study are new to the effort presented today

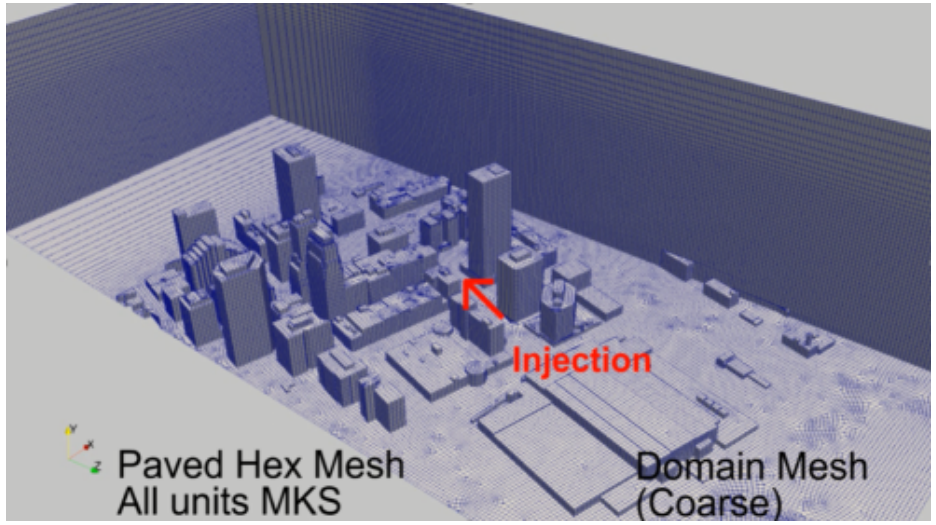
Prior Scenarios

- Prior scenarios involved comparisons to Sandia's SIERRA/Fuego CFD code
  - Comparison methods are under development
  - Model compares well, especially velocity
  - Learning how to make good comparisons to understand uncertainties

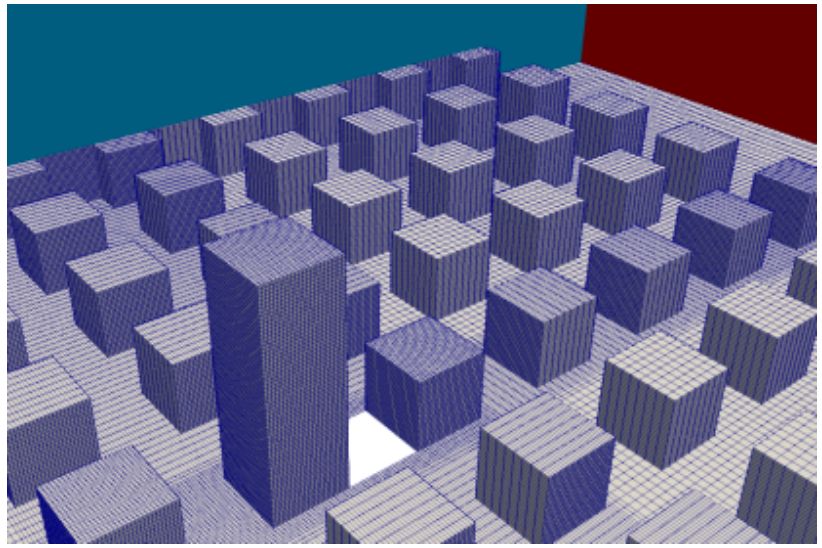
45° rotated mock urban scenario



2003 Oklahoma City



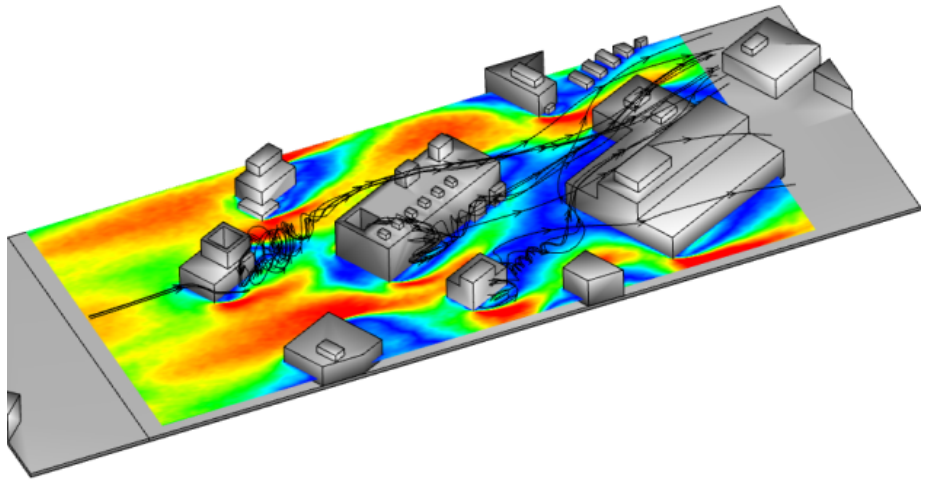
0° rotated mock urban scenario



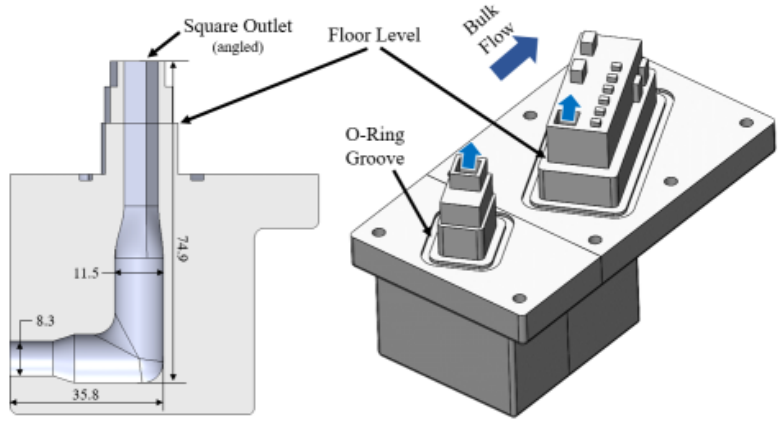
Current Scenario

- Mock urban area constructed
- Domain 4” wide, 2” high, Re: 20,000
  - Smaller than previous geometries
- Geometry 3D printed, matches CFD meshed geometry to tolerance (used identical files)

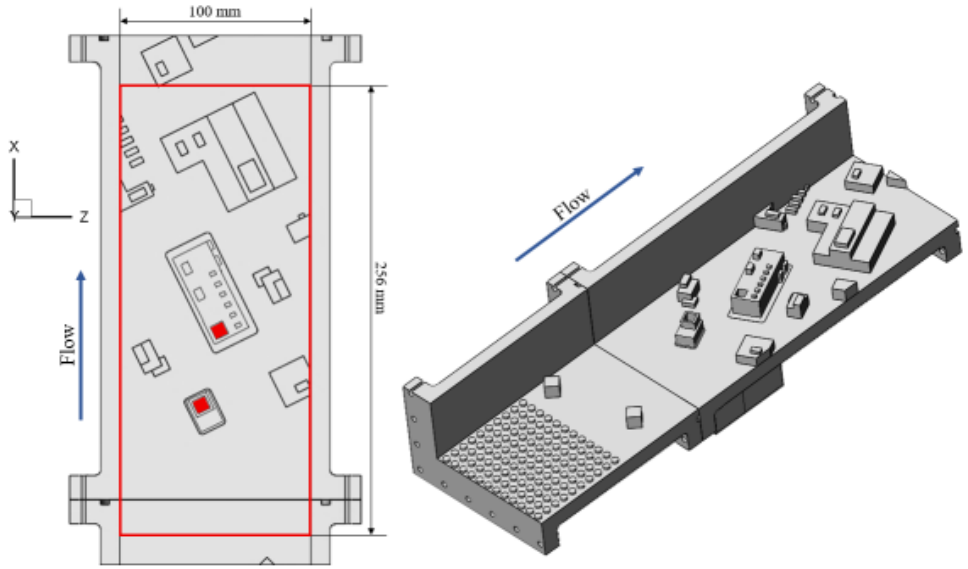
Notional geometry with data-based overlay



Inflow Boundary

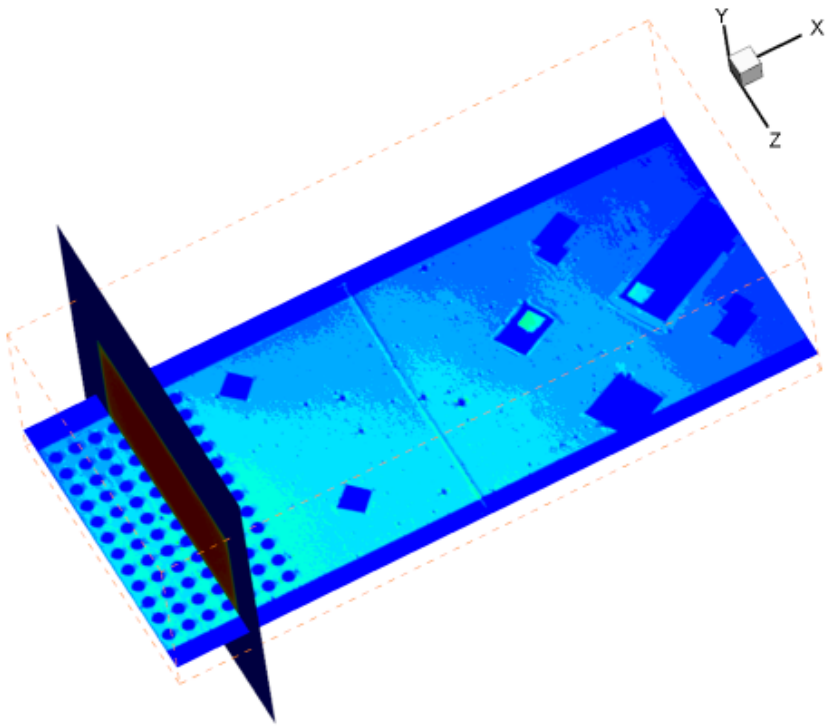


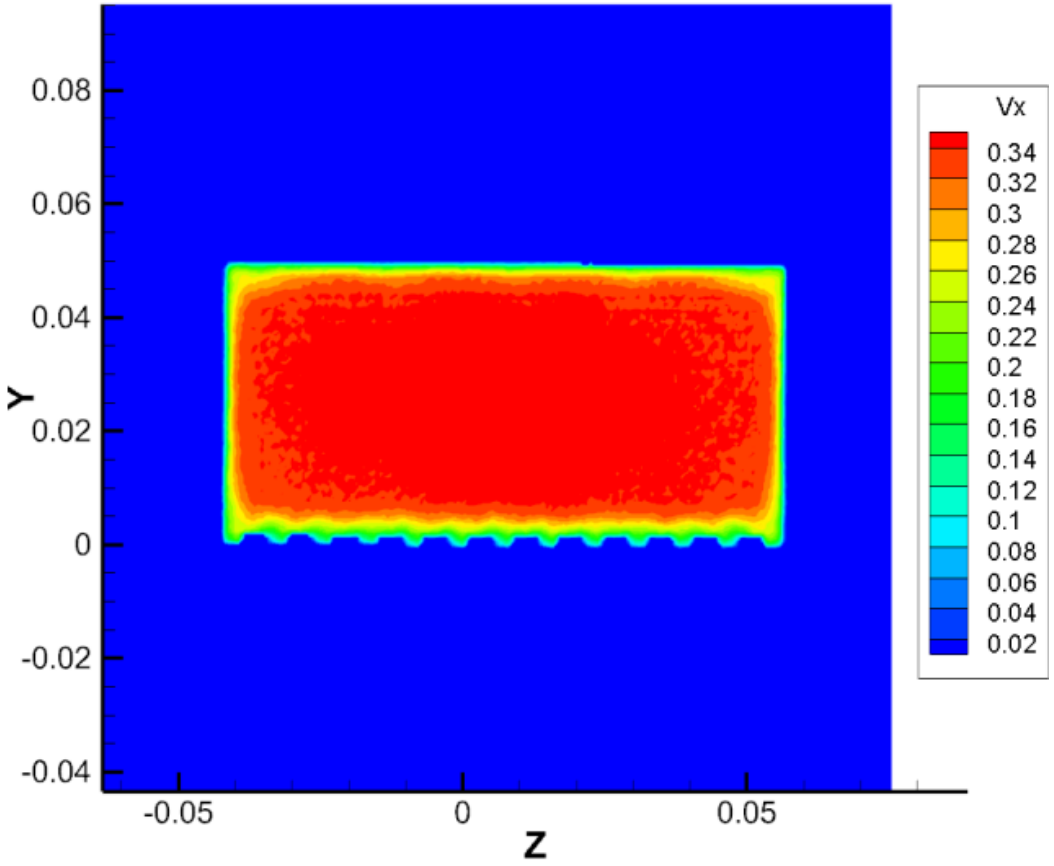
Domain



Inflow Condition

Having a 2D inflow BC is a significant benefit to the accuracy of validation comparisons with this dataset





Experimental Set-up

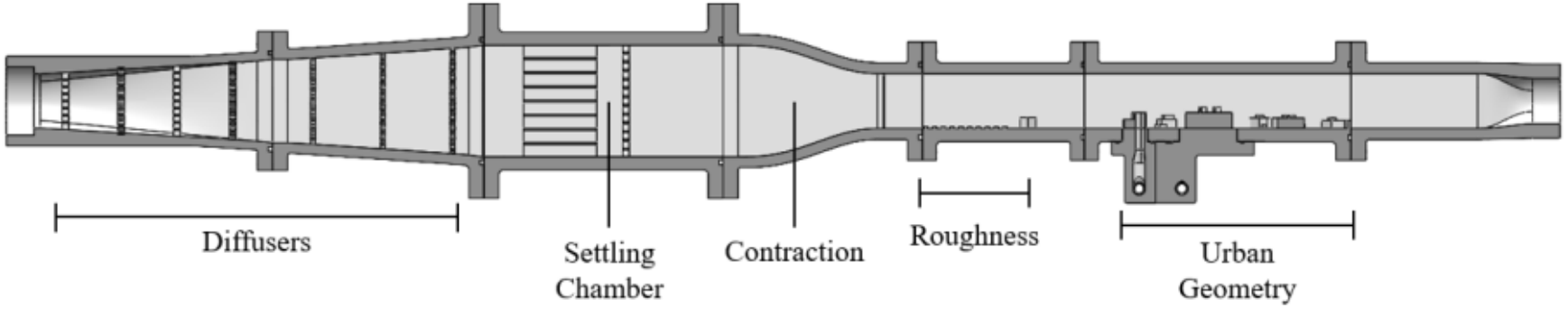
Measured mean 3-Component Velocity data by Magnetic Resonance Velocimetry

Trace $CuSO_4$ detected by Magnetic Resonance

0.6 mm resolution, millions of cells

Uncertainties around 5% of magnitude

Concentration floor of about 2.5 %



Numerical Configuration

Turbulence Models
- Large Eddy Simulation
  - KSGS

Assumptions:
- Constant Temperature, Density and Viscosity
- Buildings treated as no-slip adiabatic walls

Mixture Fraction used to study ratio of contaminant flow present in bulk flow

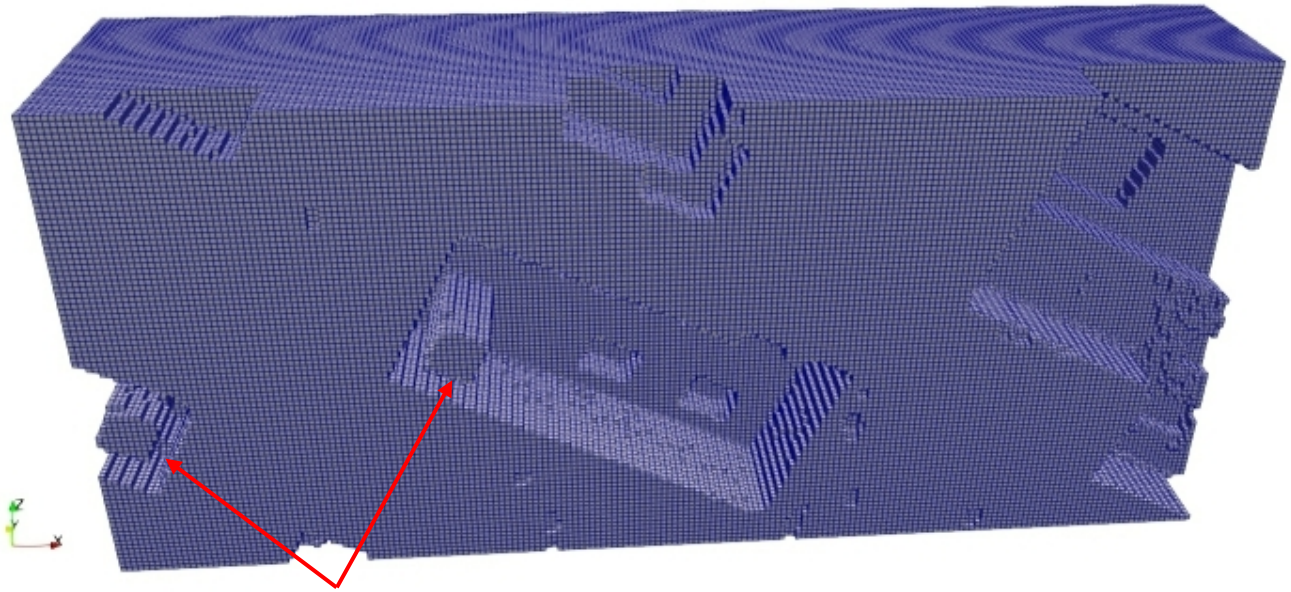
Simulations performed for 20s
- Mean velocity and concentration data collected and averaged during final 15s

Simulation results interpolated onto experimental mesh
- Smaller core plume region extracted for comparisons (as illustrated on right)

Computational Mesh Overview

Mesh	Nodes	Resolution
Coarse	482 K	1.5 mm
Medium	3.63 M	0.75 mm
Fine	12.1 M	0.5 mm

Clipped Experimental Mesh used for Comparisons



Comparison Methods

Two comparison metrics are evaluated for all data:

- Coefficient of Determination (R^2):

$$R_{xy} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})\,(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

  - Gives a measure of the linearity of the data versus model
- Euclidian Norm:

$$E_{xy} = \sqrt{\frac{\sum_{i=1}^{n}(y_i - x_i)^2}{\sum_{i=1}^{n}(y_i)^2}}$$

  - In vector space, gives an indication of the difference between the data and simulation vector magnitudes relative to the data vector

We have been evaluating many more, but we are trying to limit the number of comparisons

Results

- Simulations completed for three refinements
- Comparisons to R^2 and Euclidian Norm
  - Good comparisons on velocity magnitude
  - Concentrations compare well, could be better
- Mesh improvements not as clear as in prior scenarios
  - Slight improvement with significantly more mesh
  - Fine results not obviously better than medium

Coefficient of Determination (R^2):

Variable	Coarse	Medium	Fine
U (streamwise)	0.949	0.952	0.958
V (vertical)	0.736	0.720	0.746
W (spanwise)	0.829	0.848	0.875
Vel. Mag.	0.932	0.939	0.947
Concentration	0.910	0.934	0.922

Ideal = 1.0

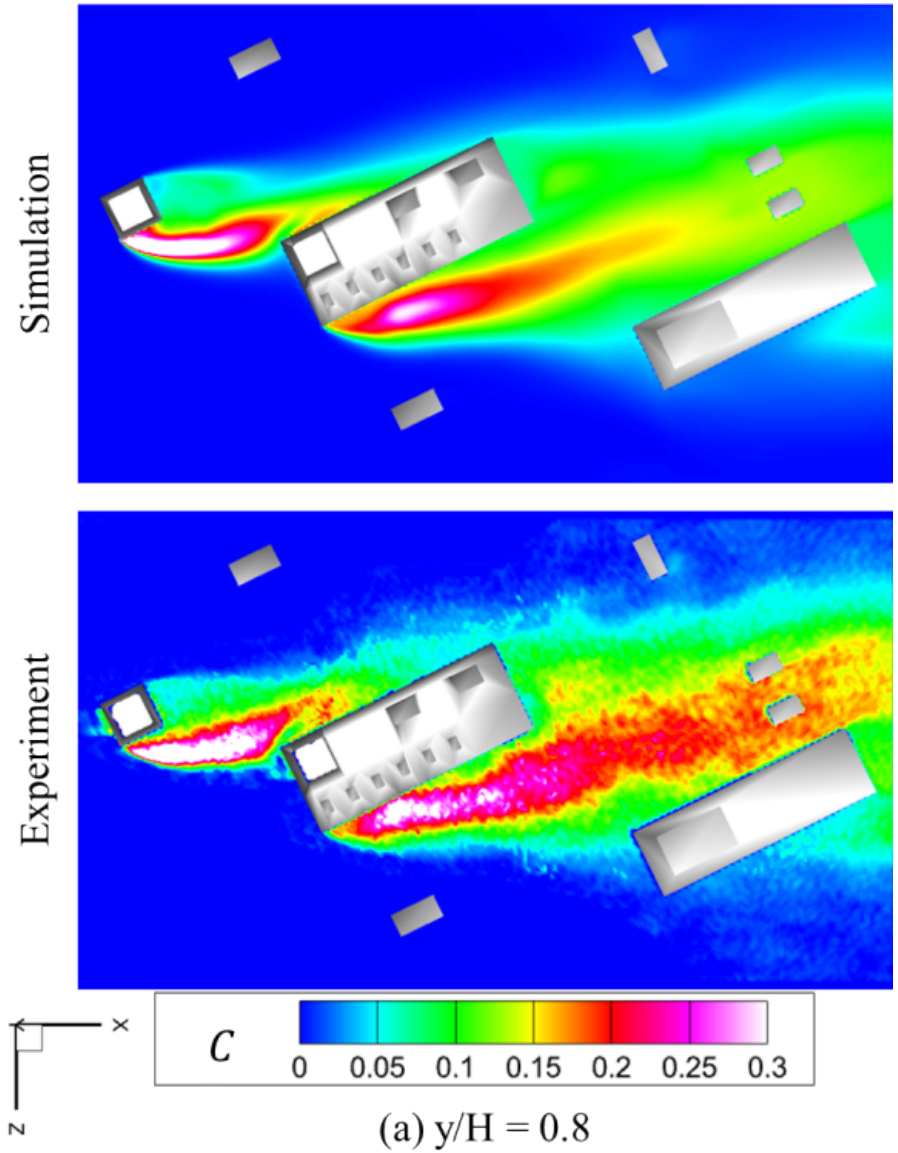
Euclidian Norm:

Variable	Coarse	Medium	Fine
U (streamwise)	0.093	0.091	0.087
V (vertical)	0.532	0.521	0.491
W (spanwise)	0.432	0.405	0.370
Vel. Mag.	0.090	0.087	0.082
Concentration	0.274	0.240	0.257

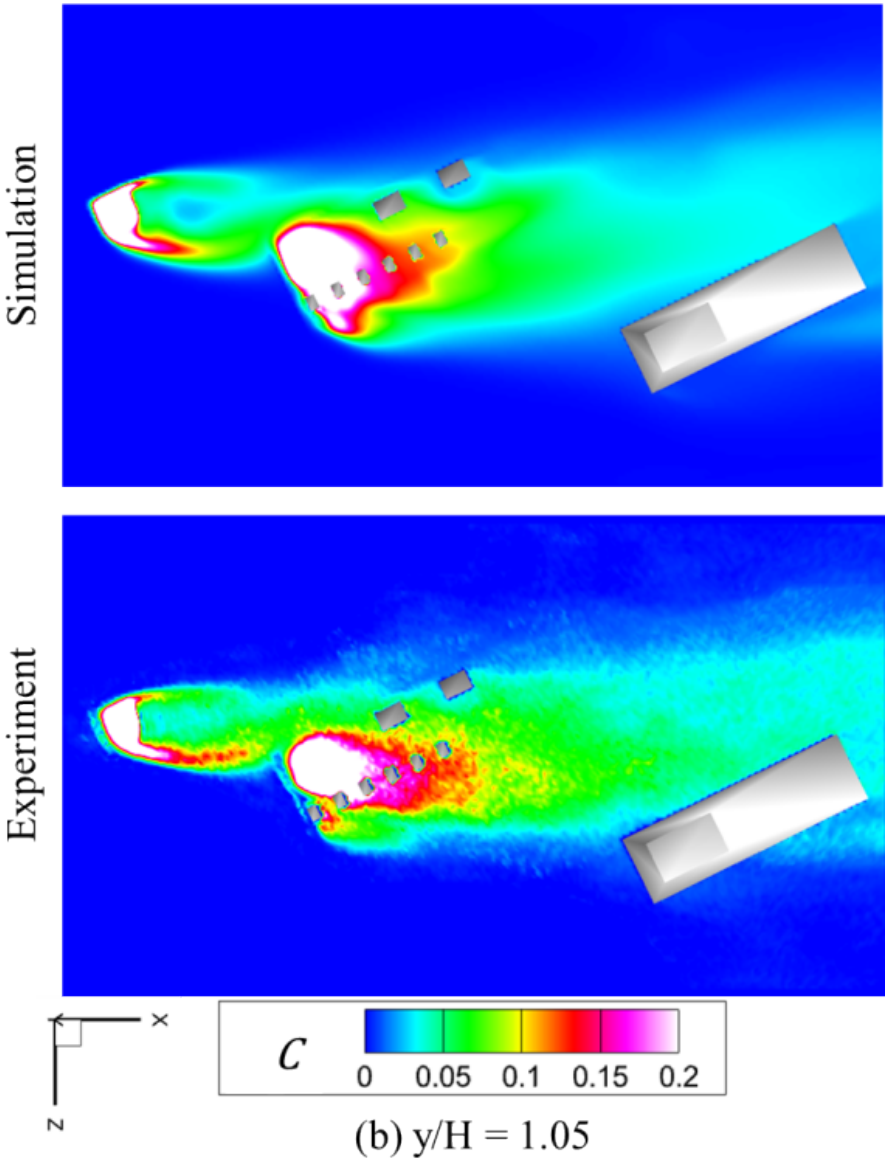
Ideal = 0.0

Concentration Contour Comparisons-medium simulation to data

- Generally good contour comparisons
- Data noise partly responsible for comparison issues
- Some localized differences



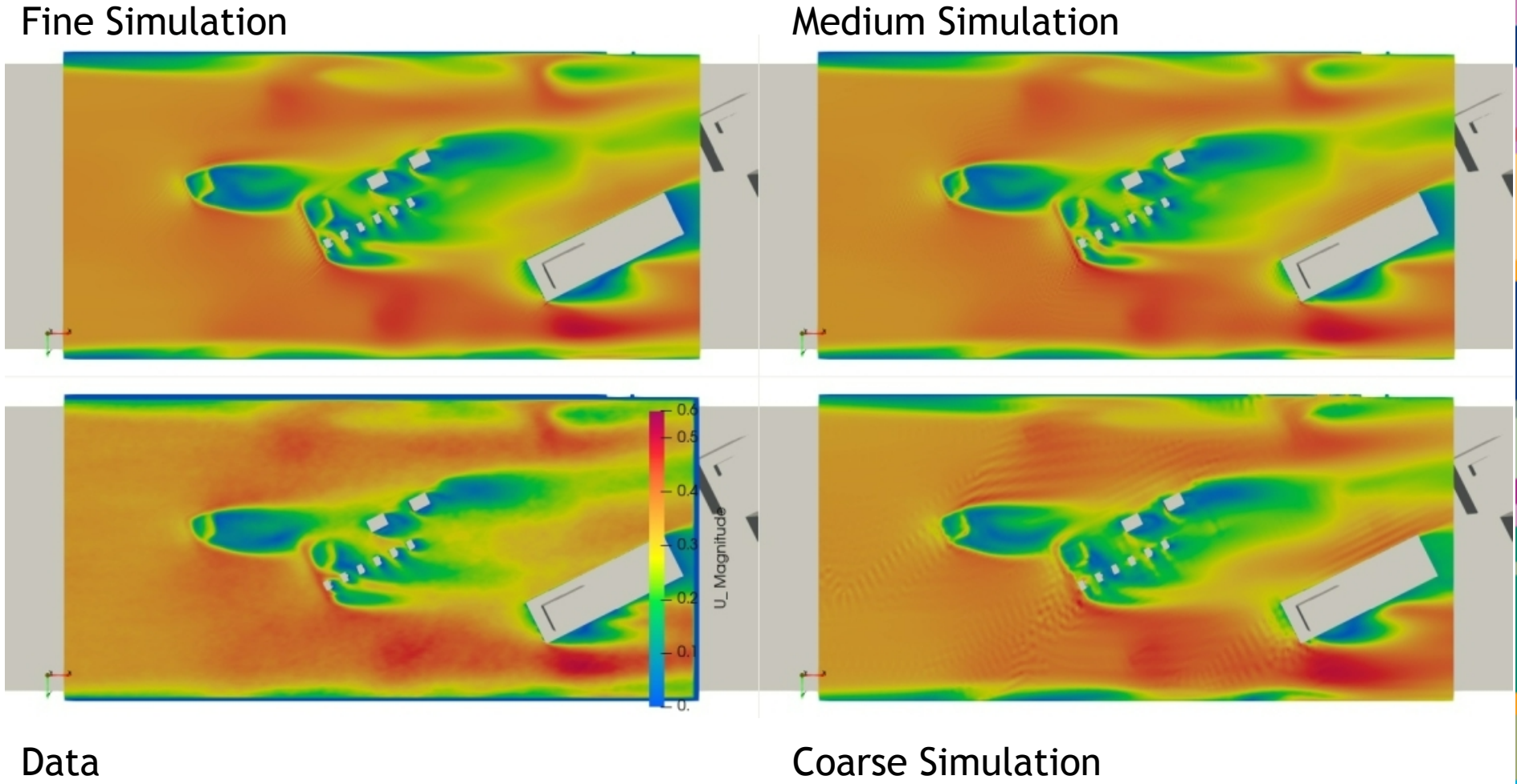
(a) y/H = 0.8



(b) y/H = 1.05

Velocity Magnitude Comparisons-Simulations to Data

- This higher elevation compares well with data
- Differences between simulations and experiment are subtle

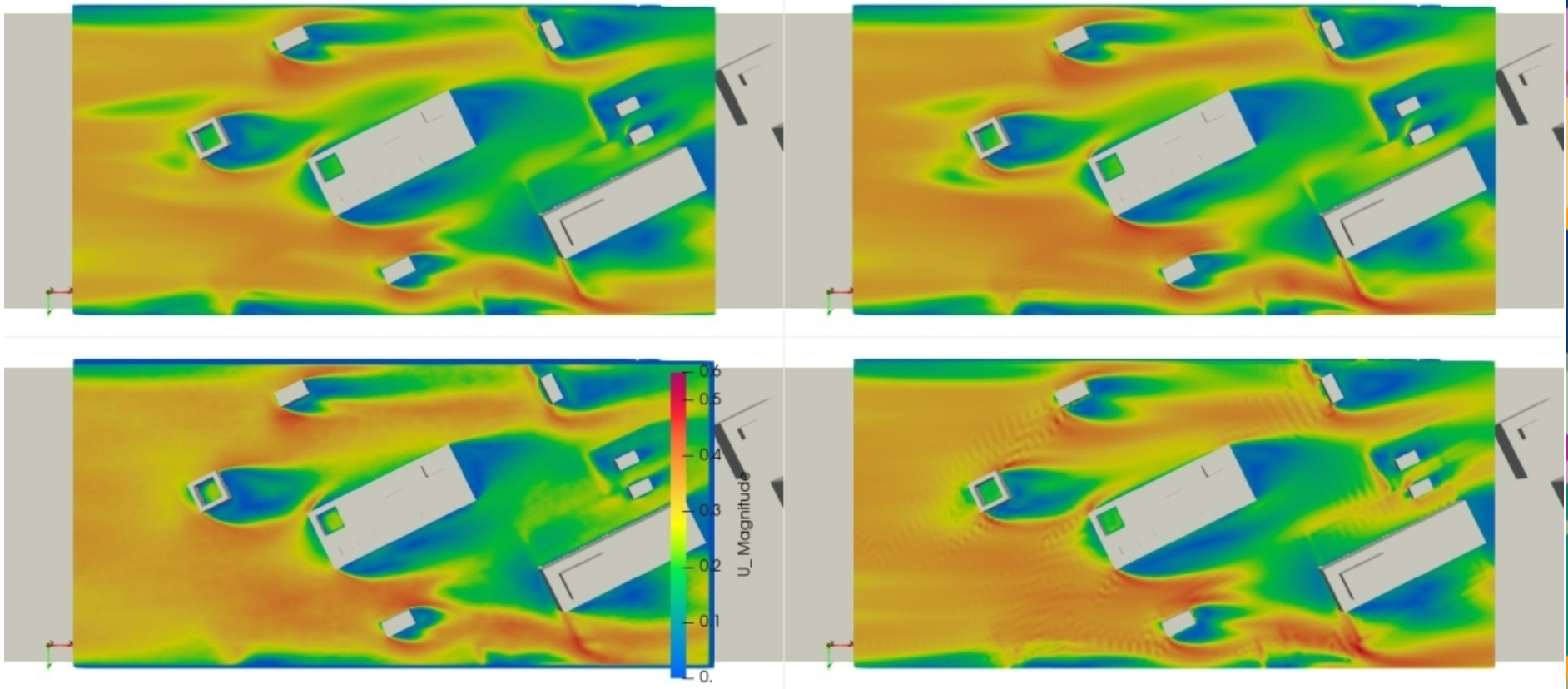


Velocity Magnitude Comparisons-Simulation to Data

- Very good comparisons at lower elevation as well
- These illustrate how close velocity magnitudes are between model and experiment

Fine Simulation

Medium Simulation



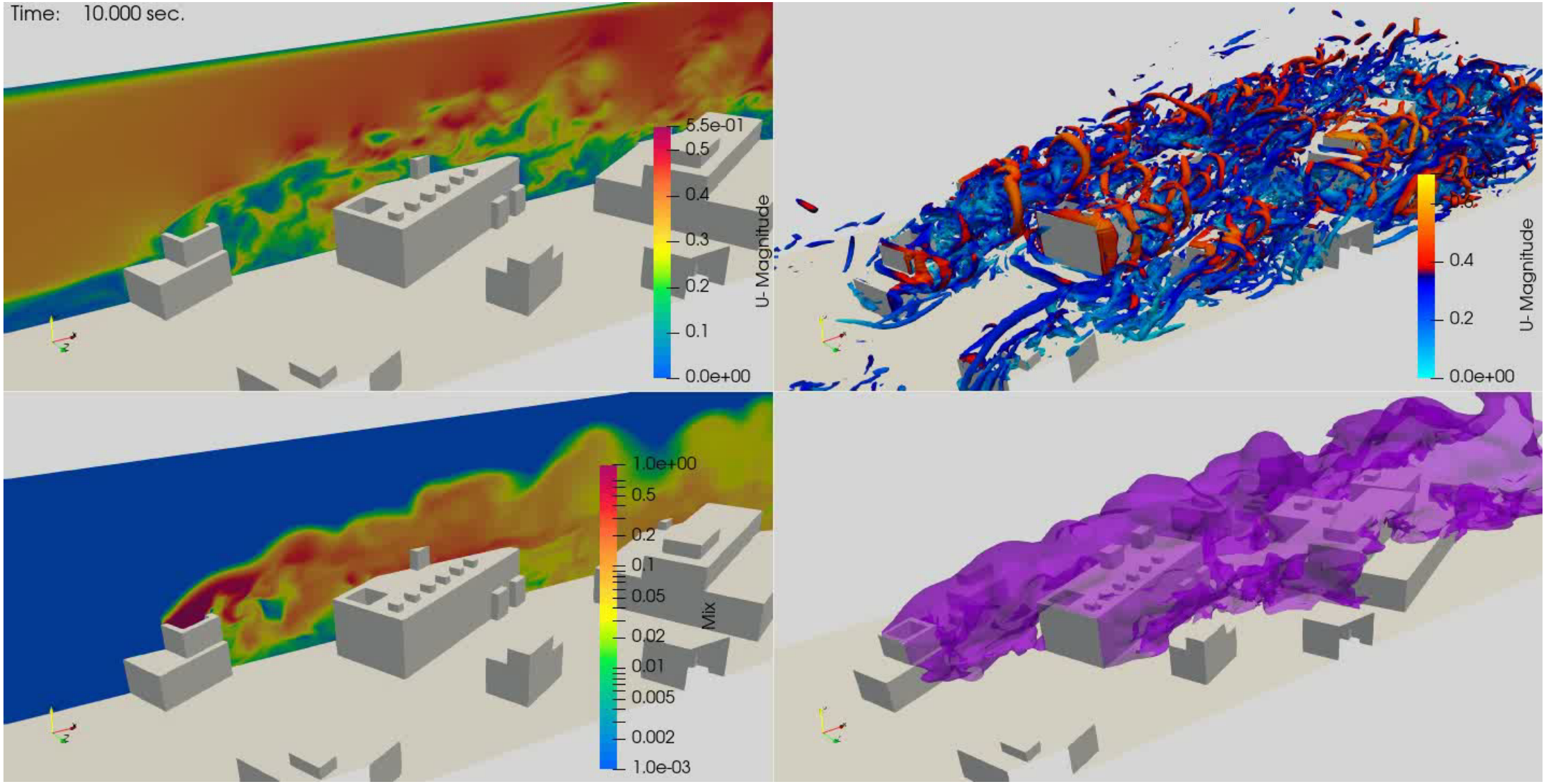
Data

Coarse Simulation

Fine Simulation Video Shows Simulated Dynamics

Velocity Contour

Q-criterion iso-contours colored by velocity

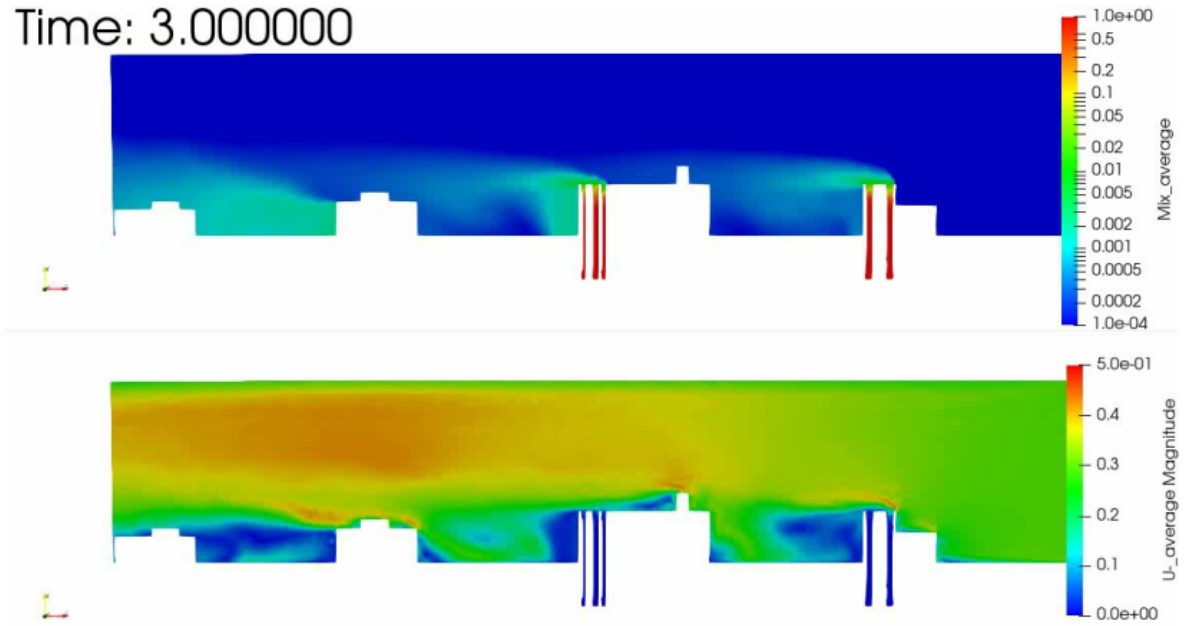


Concentration Contour

Concentration iso-contour

Future Work

- Cadets are making more extensive detailed data comparisons
- Need to focus on locations of highest error
  - These might give insight on how to improve models
- Comparison to many of the formerly used metrics in progress
- Pulsed dataset with phase resolved mean data using the same geometry
  - Data exist
  - Pre-test simulation video on right



Summary

- First 3D comparisons for simulation mesh study are exhibited here
- Euclidian Norm and Coefficient of Determination provide a concise way to assess model accuracy
  - Some differences in metric magnitudes and what they mean, but both seem to have meaningful magnitudes
- Diminishing accuracy improvements with improved CFD mesh resolution
  - Payoff of added mesh not obvious for this case
- Results quite accurate
  - Considering 5% error on data, hardly reasonable to expect better simulation comparisons for velocity magnitude
  - Comparisons poorer where measured quantities close to zero (vertical and spanwise velocities)
  - Concentration error also challenged by MRC data floor

Extras

Vorticity and Q-criterion (gradients)

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- Vorticity:

$$\vec{\omega} \equiv \nabla \times \vec{u}$$

- Useful for identifying vortices in flow (ω is vorticity, u is velocity)

- Q-criterion

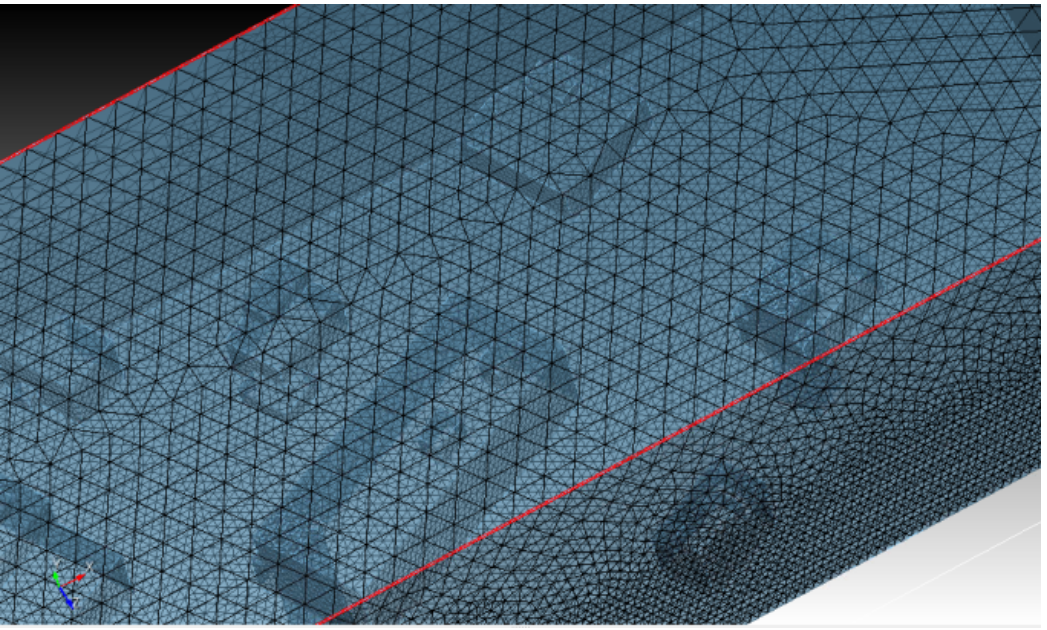
$$\overline{D_{ij}} = \frac{\partial u_i}{\partial x_j}$$

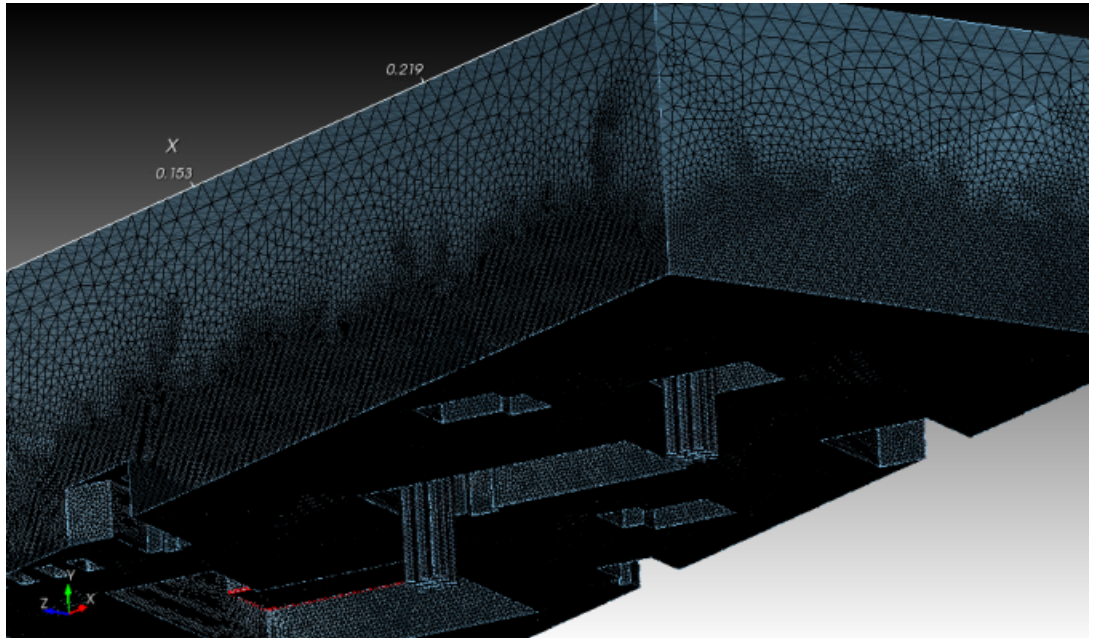
$$Q = \frac{1}{2}\left(tr(\bar{D})^2 - tr(\bar{D}^2)\right)$$

- Also helps identify vortices (eliminates shear/strain component from vorticity)
  - D_{ij} is the velocity gradient tensor, *tr* is the transpose function.
  - Hunt, J.C.R., Wray, A., Moin, P, "Eddies, Stream, and Convergence Zones in Turbulence," Center For Turbulence Research Proceedings of the Summer Program 1988, p.193.

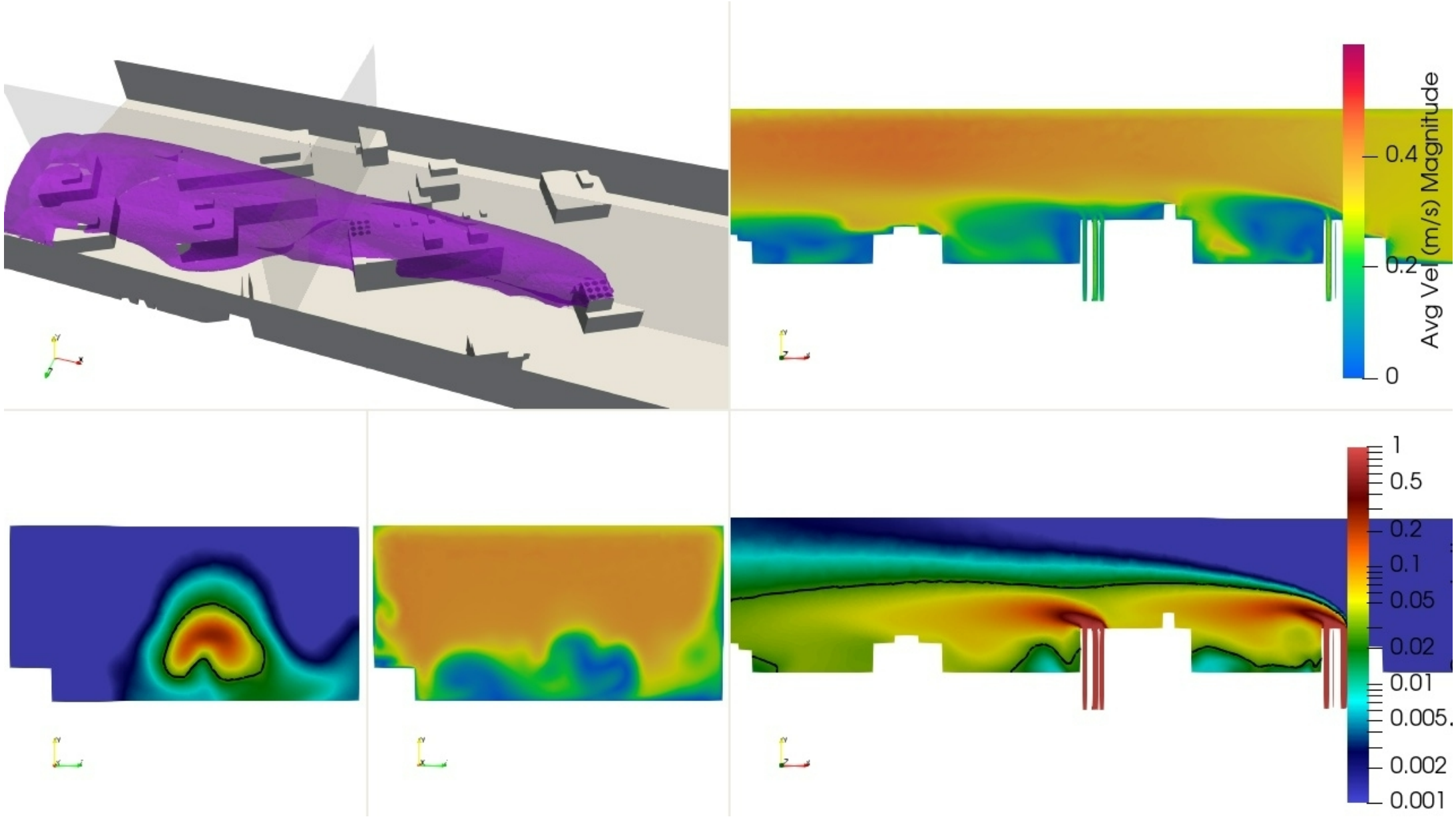
Mesh

- We are using tetrahedral mesh elements
  - They are lower quality, but meshing is very easy with tets
- Two resolutions are employed for each mesh (blends slowly between the two):
  - Coarse (at top and down-stream surfaces)
  - Fine (at buildings, ground, side walls, up-stream
- Coarse mesh has 5 mm ‘coarse’ resolution and 1.5 mm ‘fine’ resolution
- Fine mesh has 5 mm ‘coarse’ resolution and 0.75 mm ‘fine’ resolution

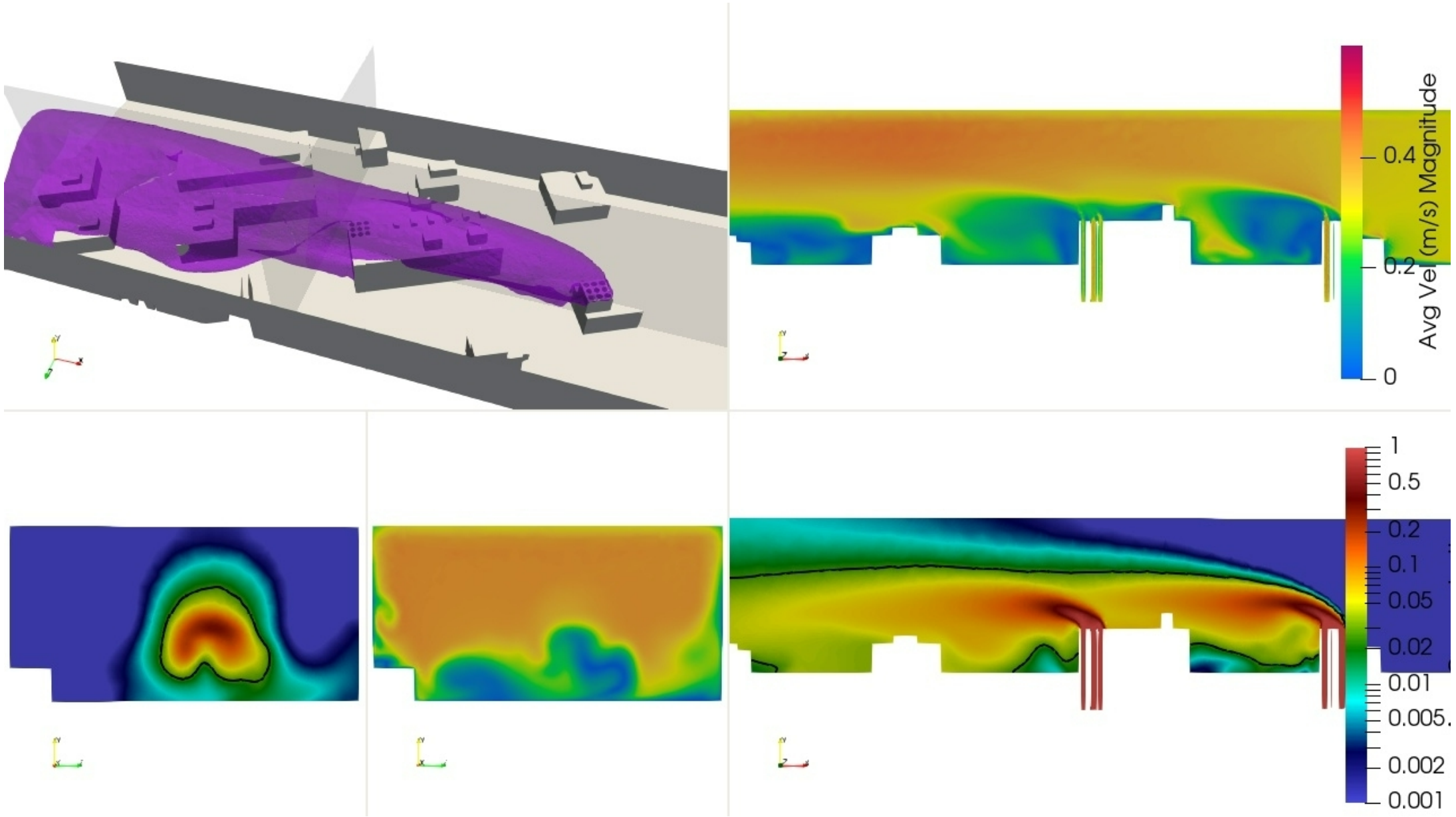




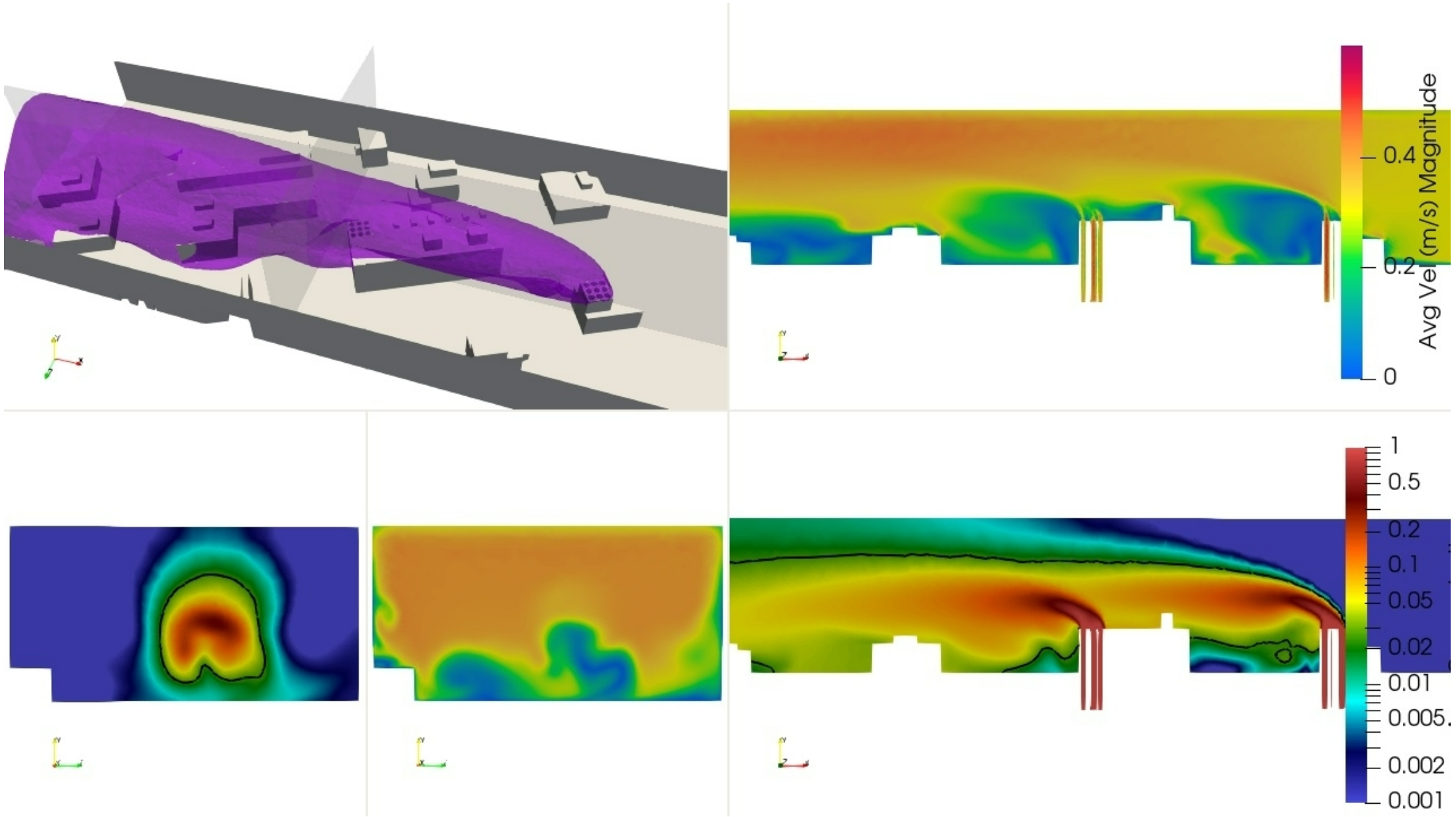
Average Results-0.3 m/s, 0.66



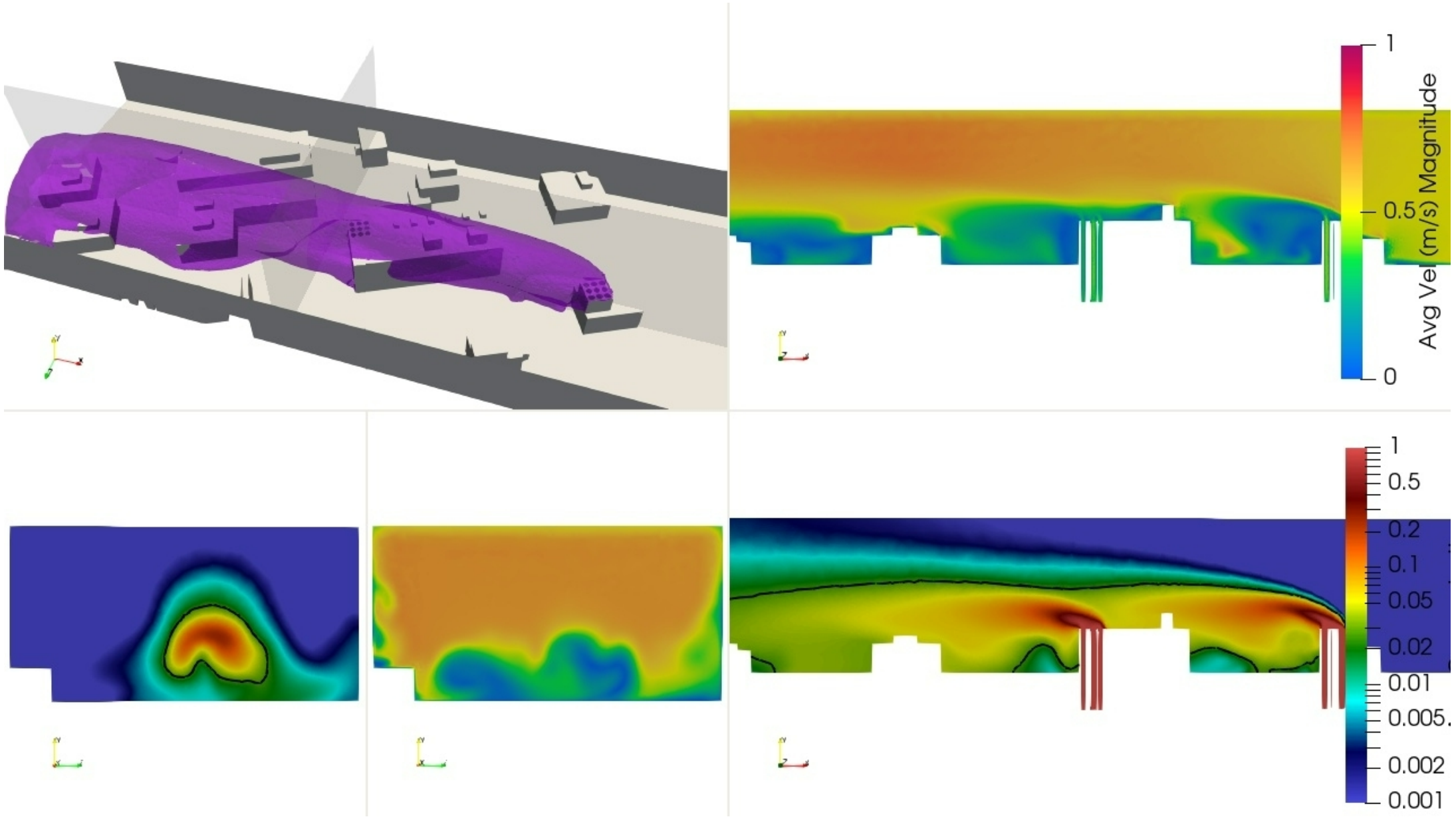
Average Results-0.3 m/s, 1.00



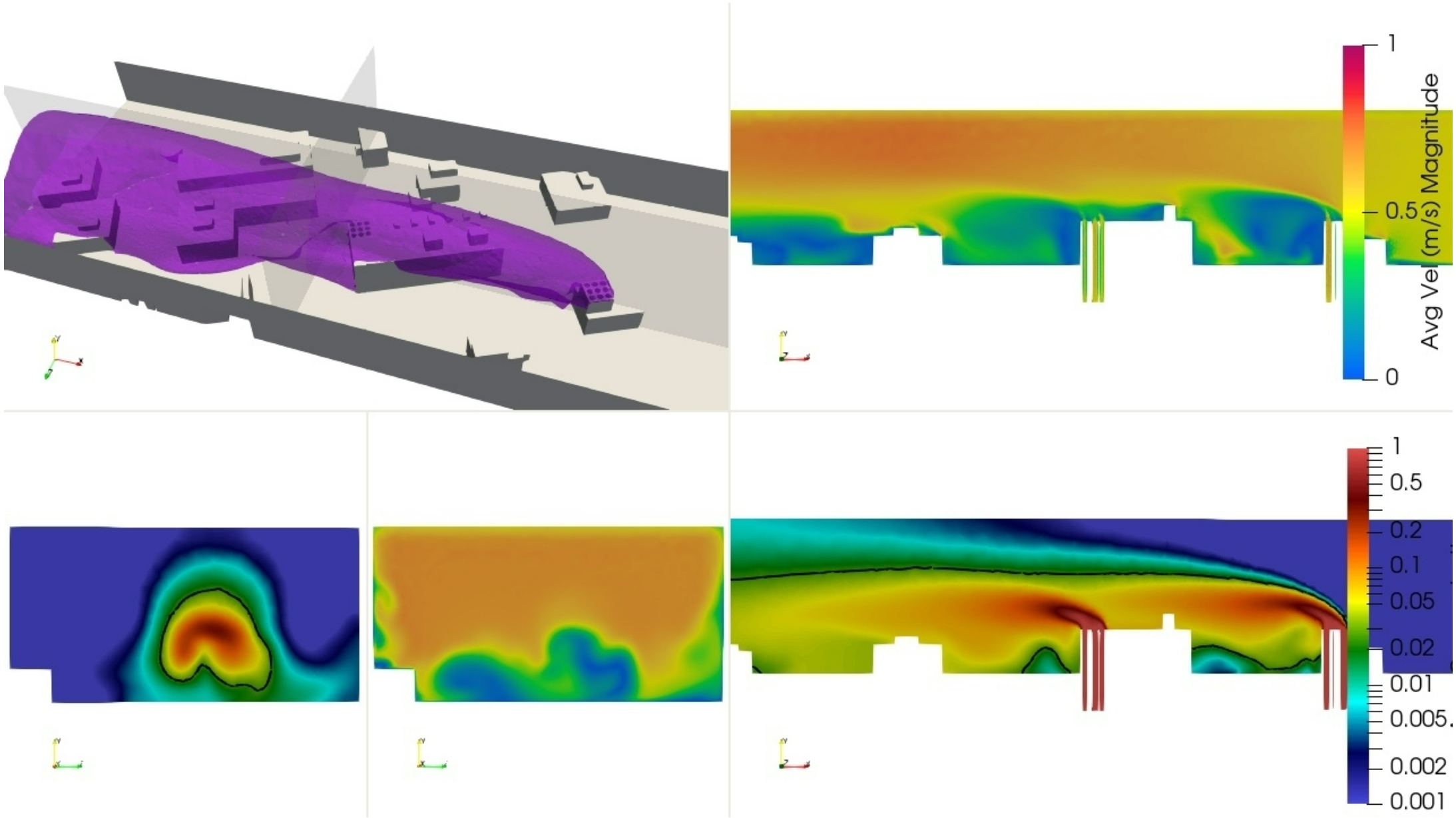
Average Results-0.3 m/s, 1.30



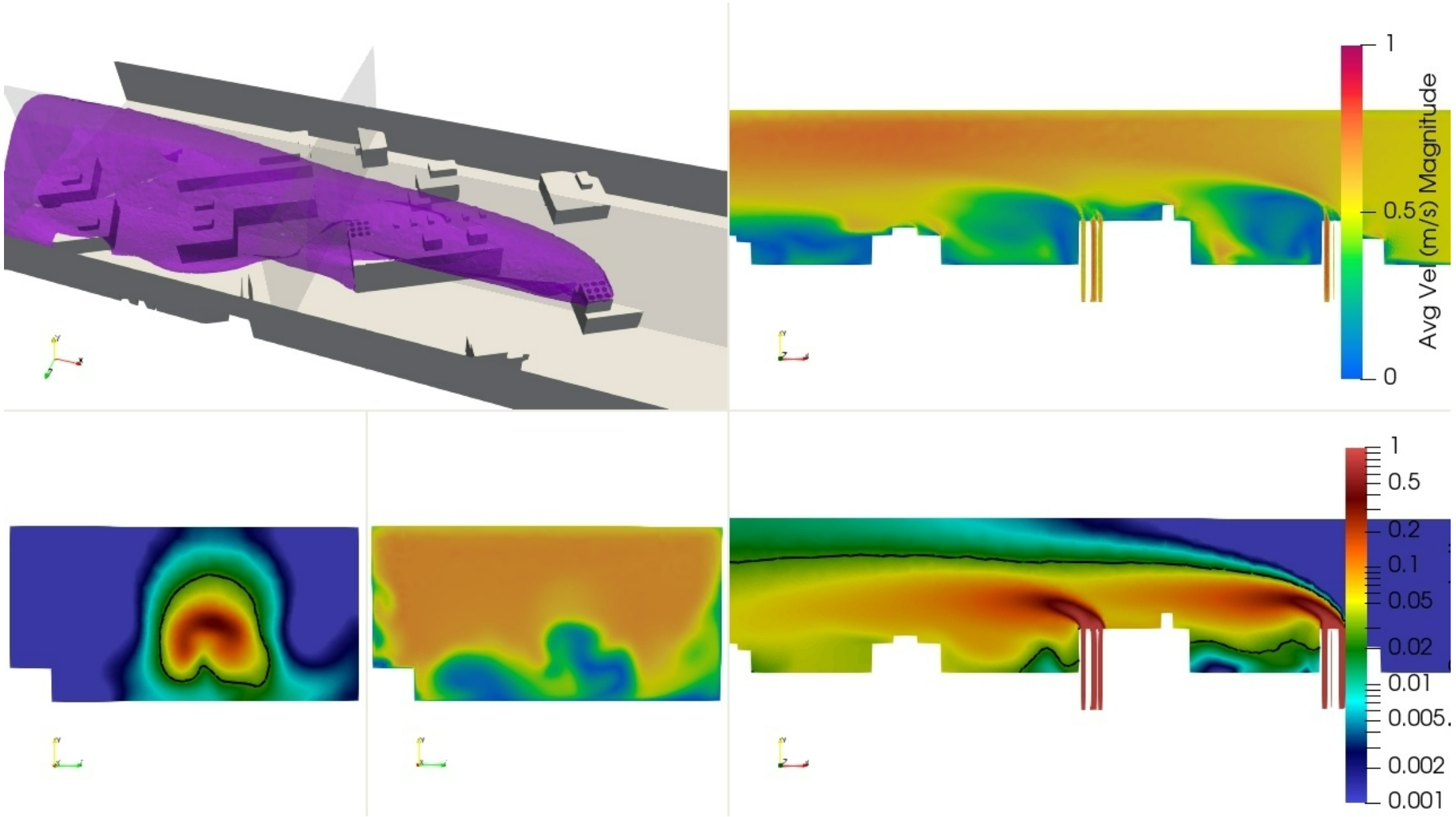
Average Results-0.5 m/s, 0.66



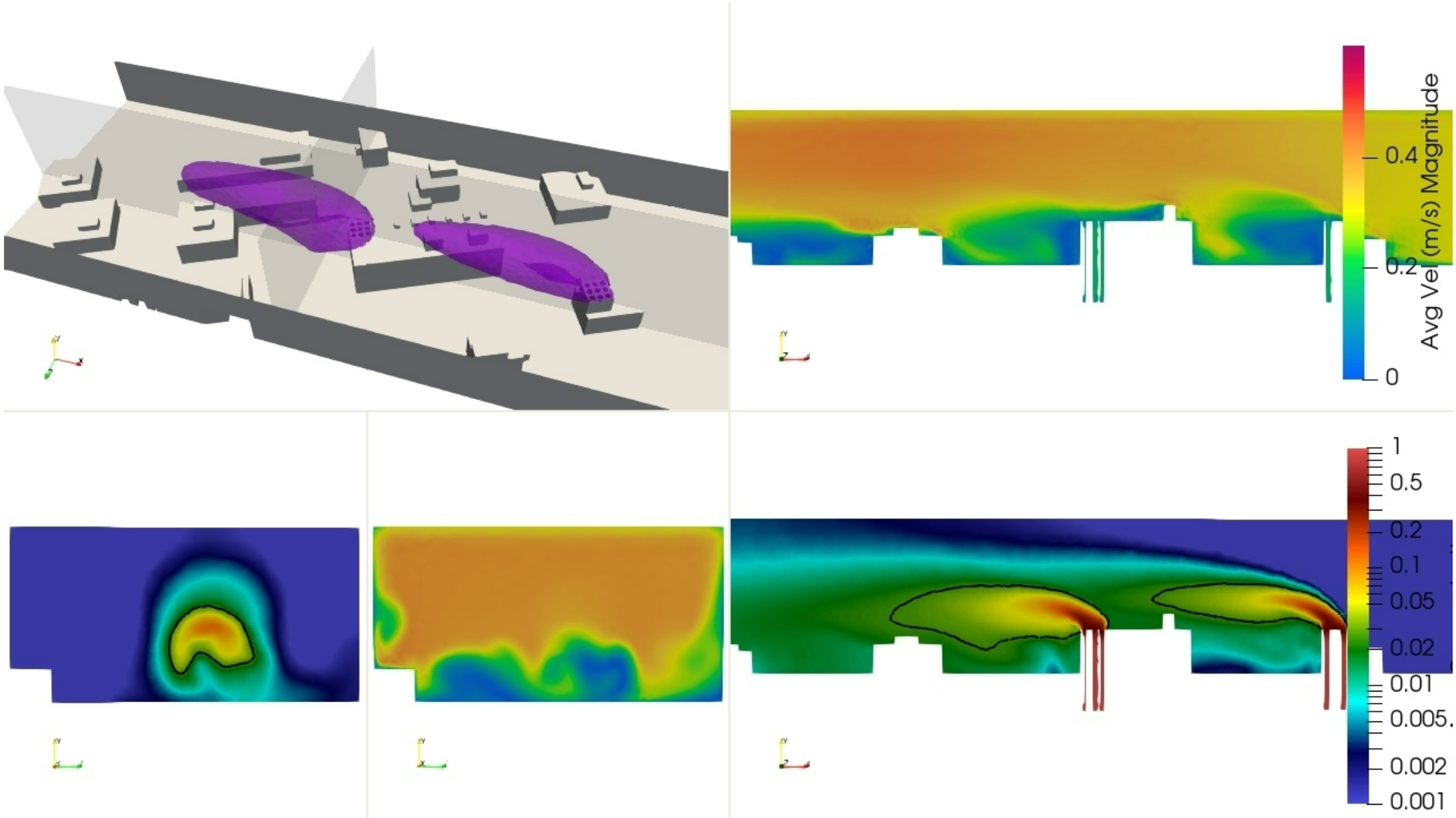
Average Results-0.5 m/s, 1.00



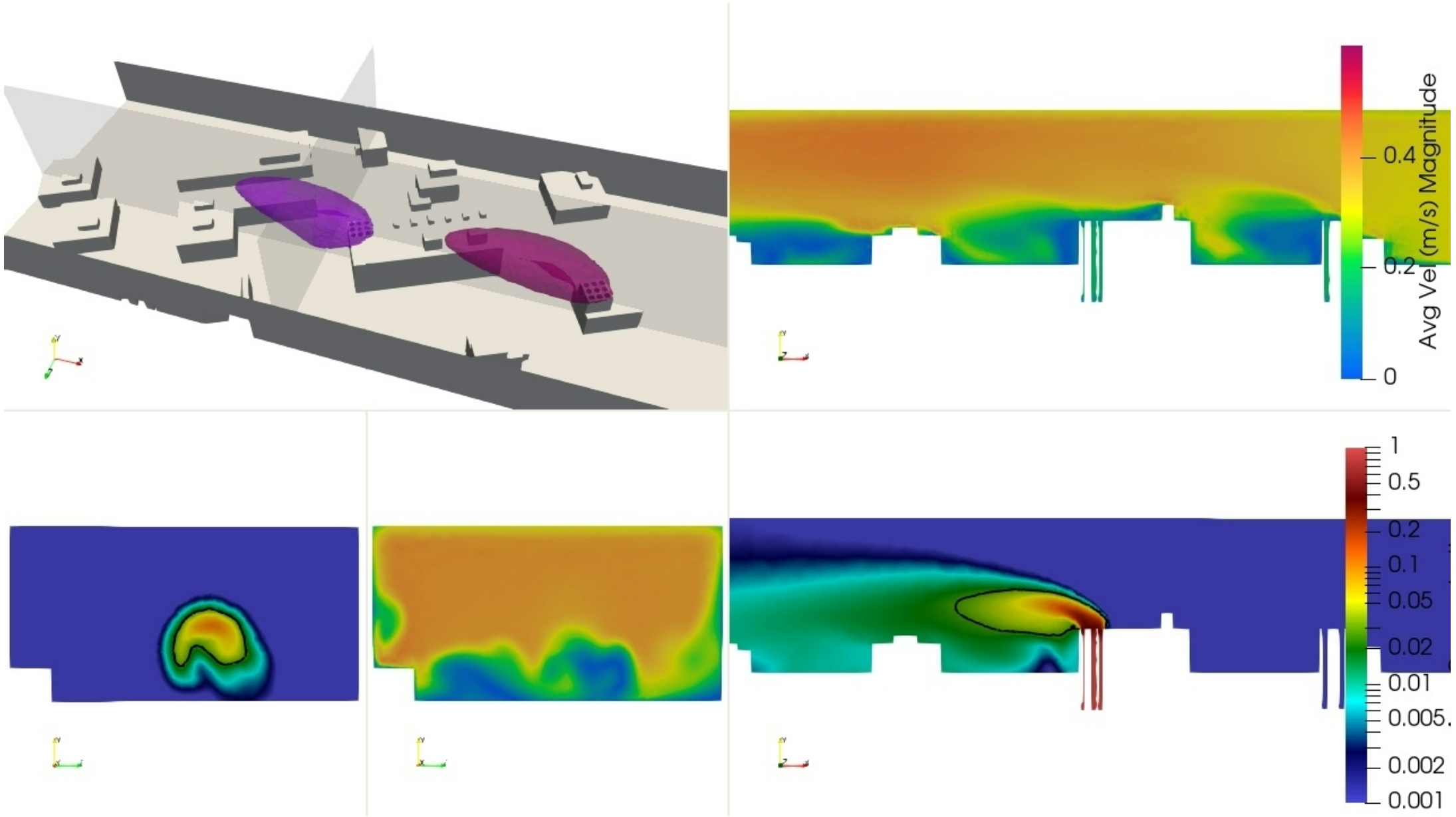
Average Results-0.5 m/s, 1.30



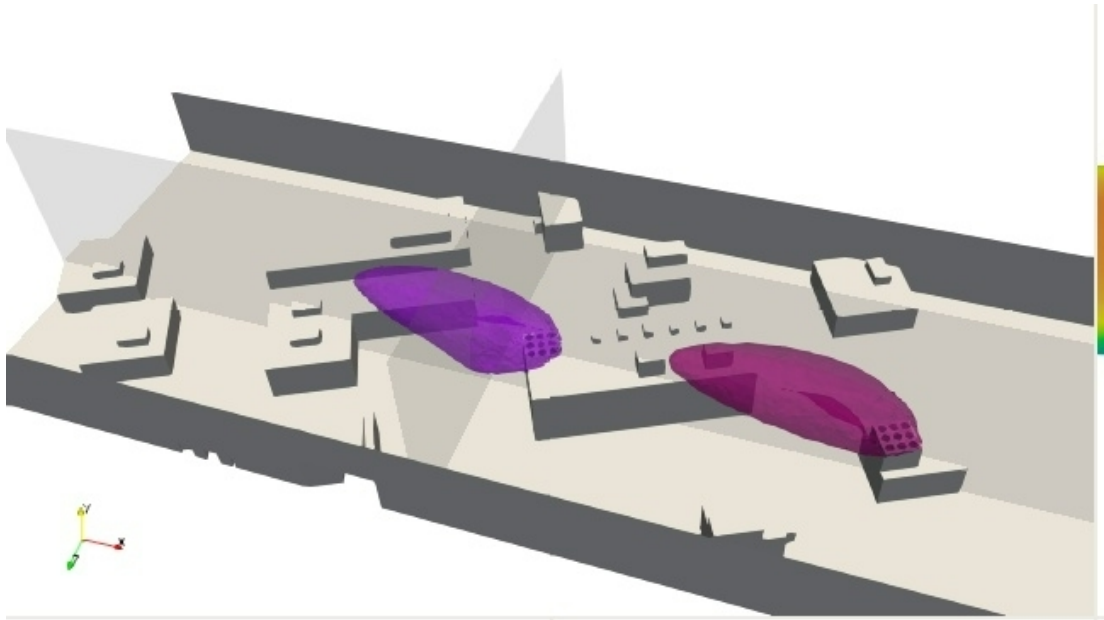
Average Results-pulsed

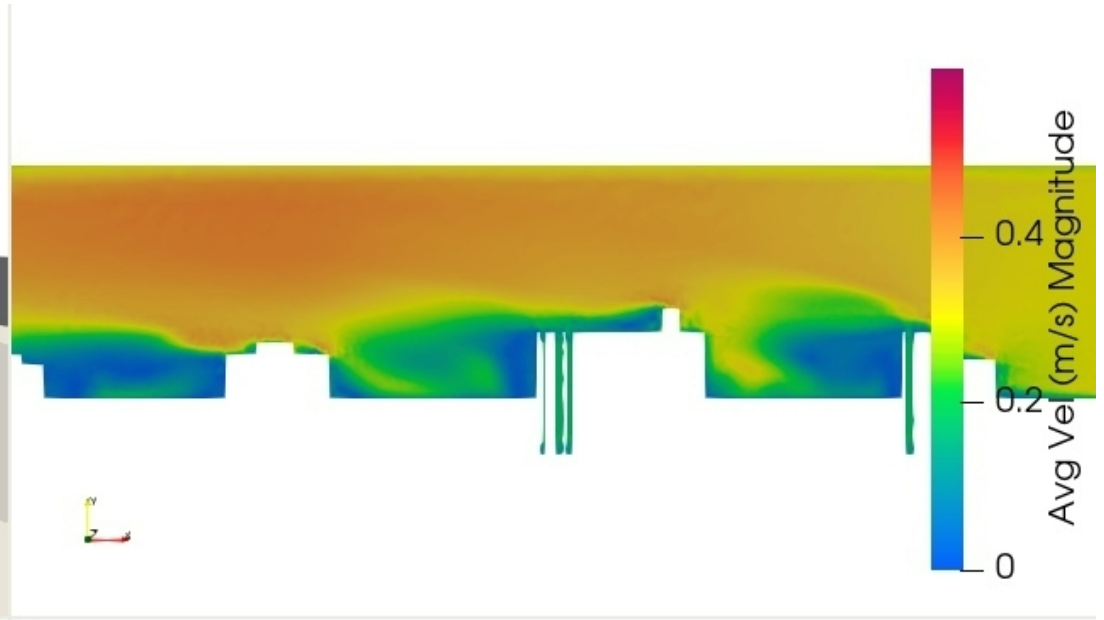


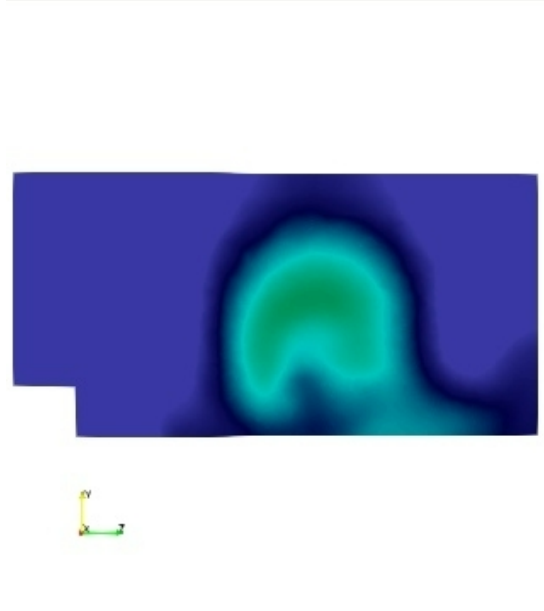
Average Results-pulsed, 2 mixture fractions

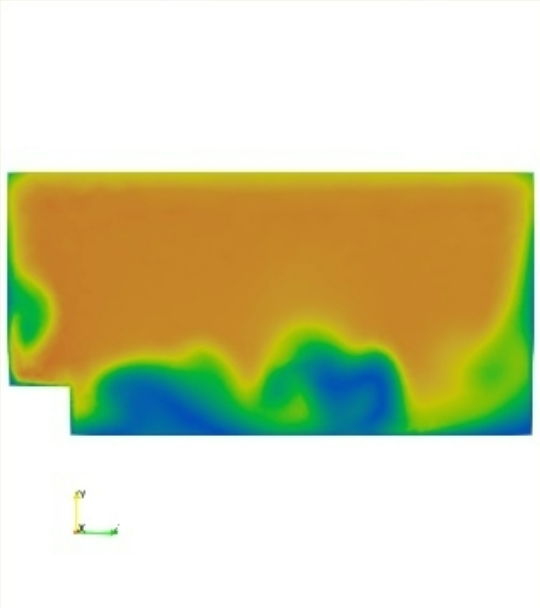


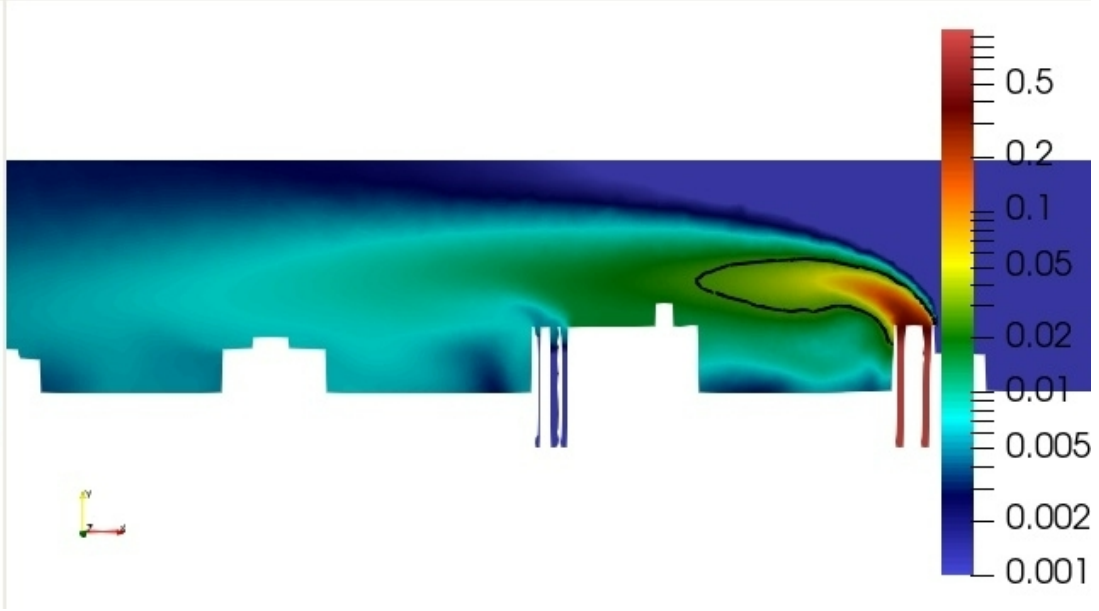
Average Results-pulsed, 2 mixture fractions-second mix-frac



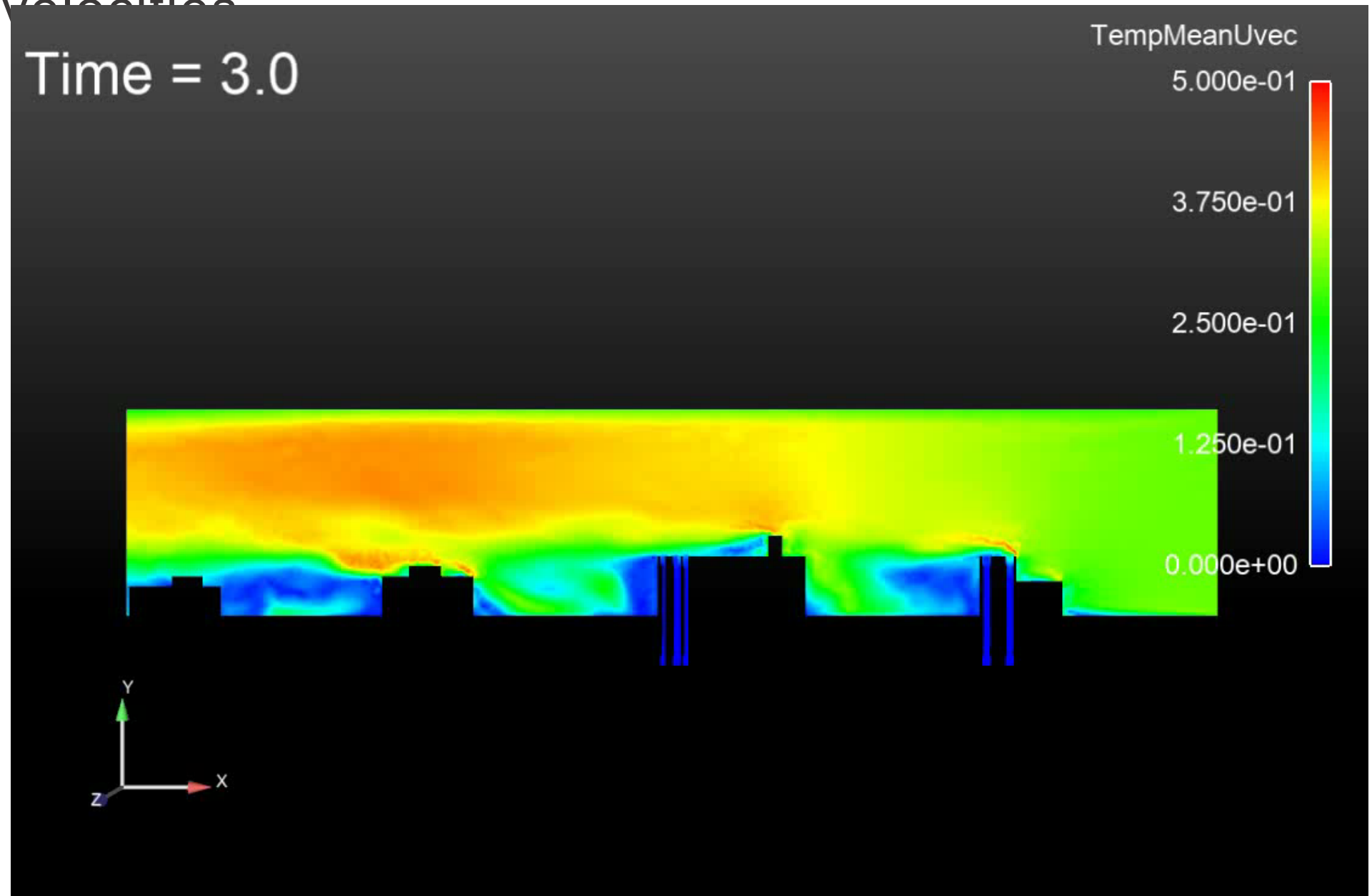




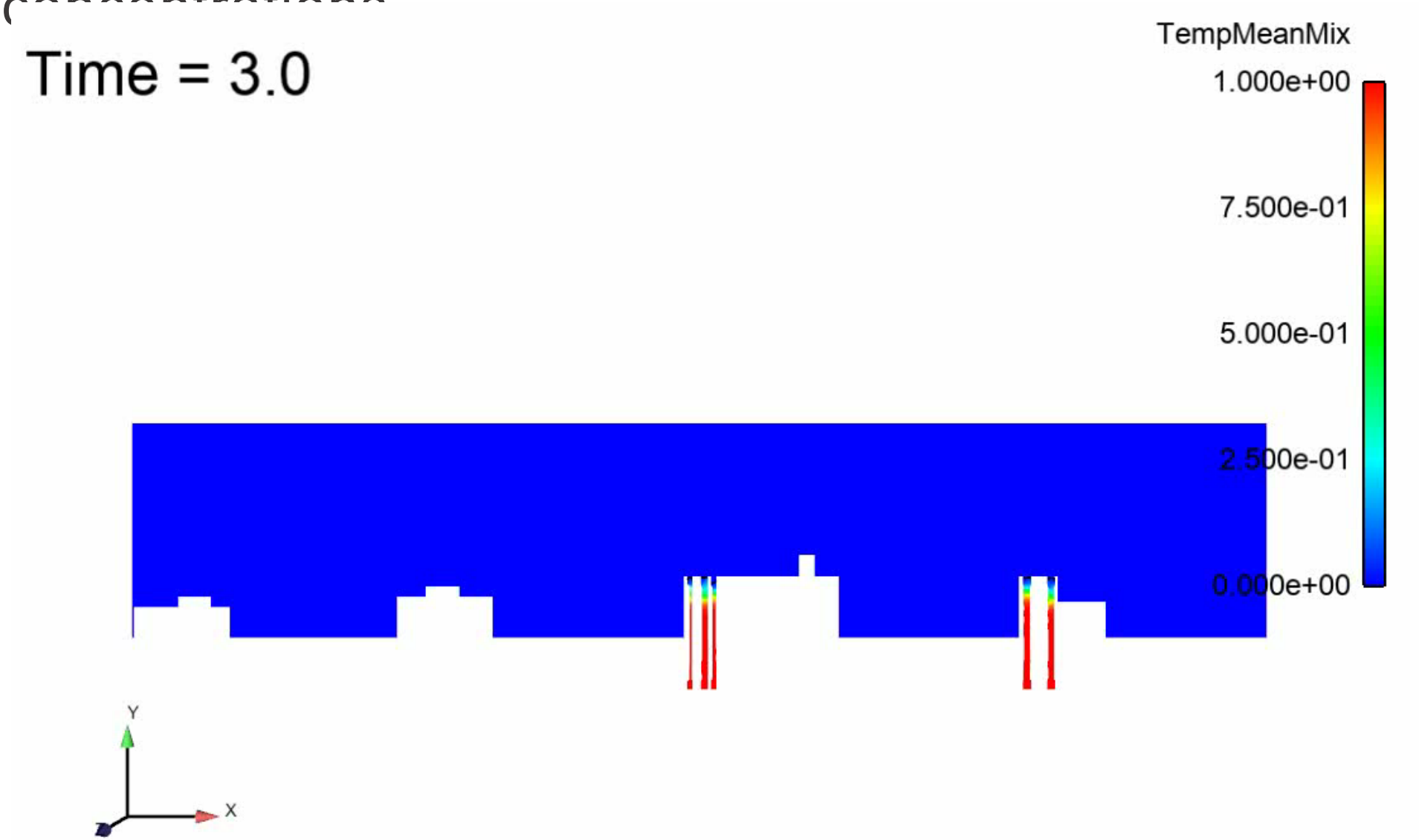




Phased Results-Average (60 seconds, 20 cycles) pulsed velocities



Phased Results-Average (60 seconds, 20 cycles) pulsed concentrations



Phased Results-Average (150 seconds, abt 50 cycles) pulsed concentrations