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Detailed 3D flow and concentration methods and validation with MRC/MRV techniques I

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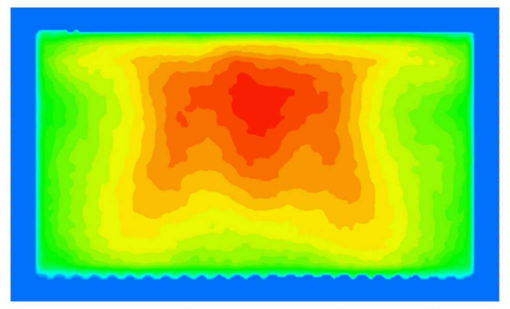
Abstract

The techniques of Magnetic Resonance Concentration and Magnetic Resonance Velocimetry have been applied to a series of flow conditions motivated by scenarios of interest to the plume transport community. The techniques employ scaled water flow as a surrogate for air and provide 3-dimensional velocity vector and concentration data throughout the measurement domain for a turbulent flow ($Re \approx 10^4$). This approach makes possible validation comparisons between data and model that are unprecedented in detail and scope, with hundreds of thousands of comparison points. They also challenge the traditional validation methodologies that typically lack the fidelity of information available for data and models. This poster focuses on what we call the 90 degree scenario that involves a regular array of cubic mock buildings (H being the size of the buildings as well as building spacing) with a single large structure (3H in height). This case is previously studied in the flow and dispersion communities and represents a challenging urban scenario for dispersion models. This paper focuses on the initial 3-D comparisons between models and data. Some prior work provides guidance on how to make comparisons in this environment, and some new techniques and approaches are detailed that are used for this comparison. This paper exhibits techniques for comparing the velocities and concentrations in the full domain for several characteristic cut-planes, and for a large volumetric region where the simulated concentration is above 0.025 mass fraction. The data compare well with the model, and quantitative measures of the accuracy are presented. This work provides benchmark accuracy metrics for SIERRA/Fuego and also provides guidelines on recommended methods for subsequent comparisons of this nature. Parameter relations are deduced using a correlation analysis. Quantitative results depend lightly to moderately on the method used to down-select the comparison data. The magnitude of this is shown. Use of cut-planes can be an effective data reduction technique.

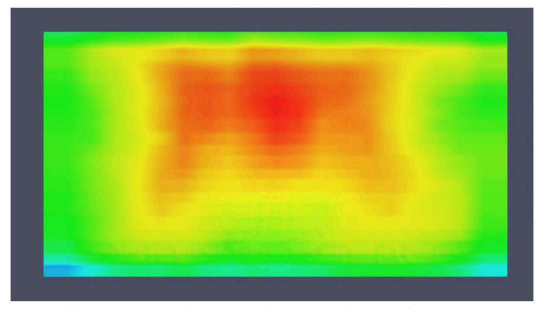
Methods

The MRI at Stanford university is used to make **flow and dispersion measurements** for canonical flow conditions

Measured Inflow

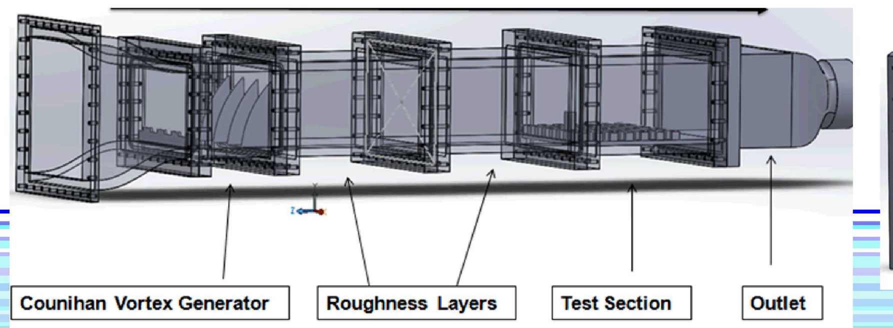


Modeled Inflow

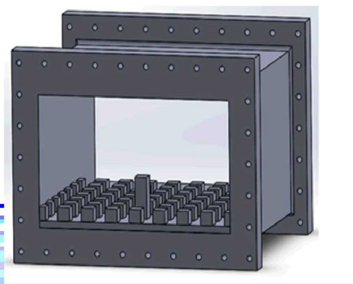


Additive manufacturing is used to construct the water channel, injectors, and flow surfaces (Stanford/USMA)

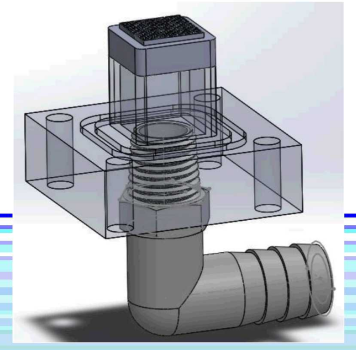
Channel



Test section

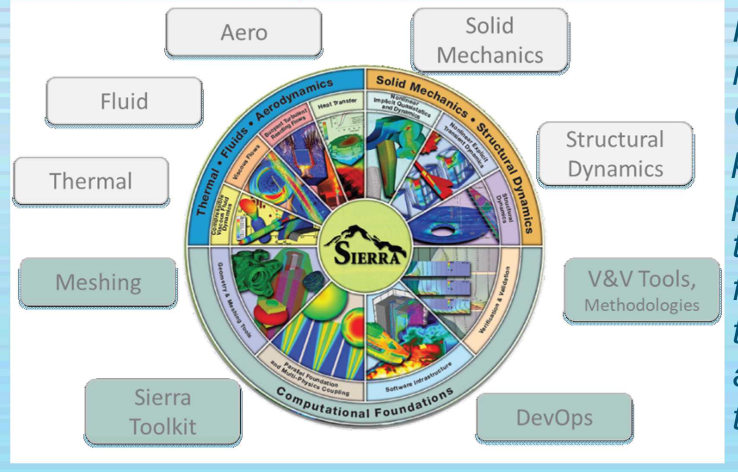


Injector

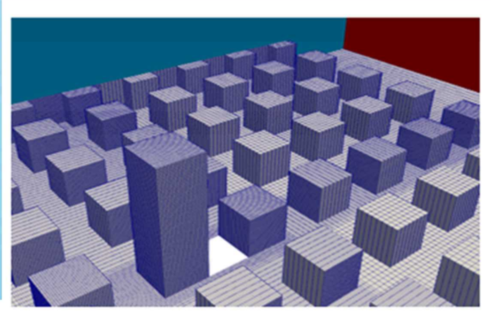


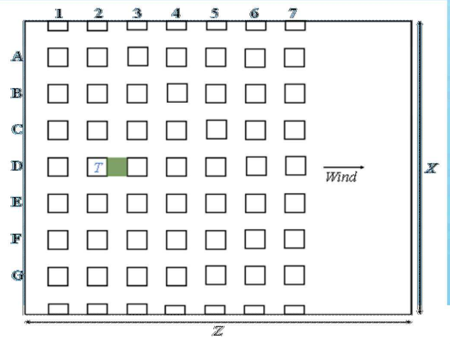
SIERRA/Fuego is used to simulate the scenarios (Sandia)

SIERRA is a computational framework for solving engineering applications on massively parallel architectures. SIERRA applications are used by the US Energy, the Defense Department and others for solving complex engineering analysis and design problems.



Fuego is the low-Mach number fluid mechanics CFD capability used for fires, plumes, heat transport, particles, multiphase transport, etc. This work focuses on applying Fuego to a plume transport problem and validation of the code for that application.





Simulation mesh (far left) and drawing of the building layout (left) with coordinate system, column and row designations for identifying the locations of planes and points in the domain. The block labeled T is for the tall building.

Methods (continued)

This comparison work was initially guided by the approach Hanna and Chang (2012)** proposed for comparing campaign-level test results to simulations. They proposed the following metrics for assessing performance of computational models:

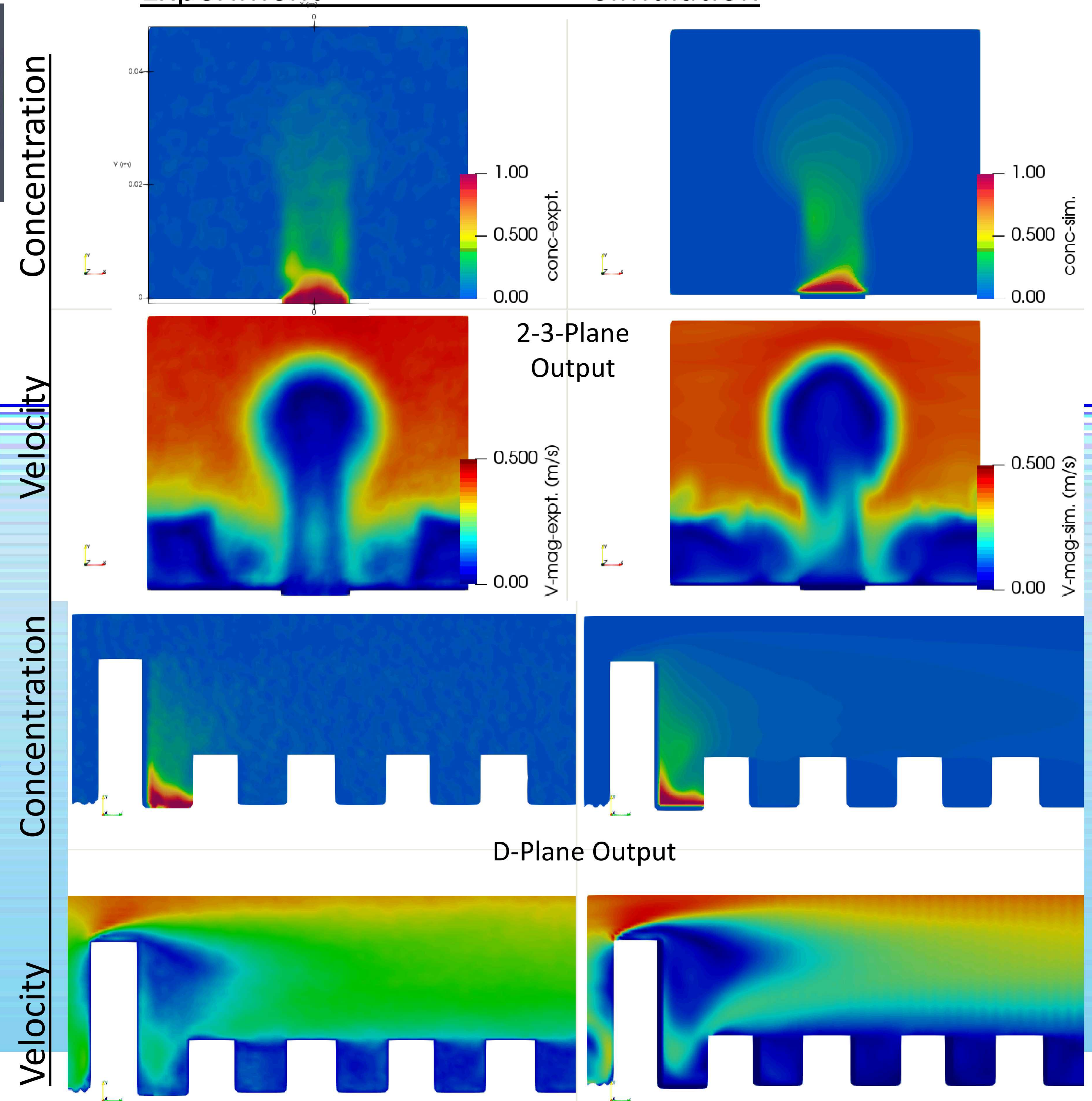
- The Fractional Mean Bias (FB): $2\left(\overline{C_o - C_p}\right)/\left(\overline{C_o} + \overline{C_p}\right)$
- The Normalized Mean-Square Error (NMSE): $\left(\overline{(C_o - C_p)^2}\right)/\left(\overline{C_o} \times \overline{C_p}\right)$
- The Geometric Mean (MG): $exp\left(\overline{lnC_o}\right) - exp\left(\overline{lnC_p}\right)$
- The Geometric Variance (VG): $exp\left(\overline{(lnC_o - lnC_p)^2}\right)$
- The Fraction of Predictions with in a Factor of 2 of the Observations (FAC2): 0.5<(Cp/Co)<2
- The Normalized Absolute Difference (NAD): $\left|\overline{C_o - C_p}\right|/\left(\overline{C_o} + \overline{C_p}\right)$

They propose an urban acceptance criteria of |FB| < 0.67; NMSE < 6; FAC2 > 0.3; and NAD < 0.5 for concentration data (c_p being the predicted variable and c_o being the observed). We also introduce:

$$LND = \frac{|C_p - C_o|}{max(C_p, C_o)} \qquad LLR = ln\left(\frac{max(C_p, C_o)}{min(C_p, C_o)}\right)$$

Results

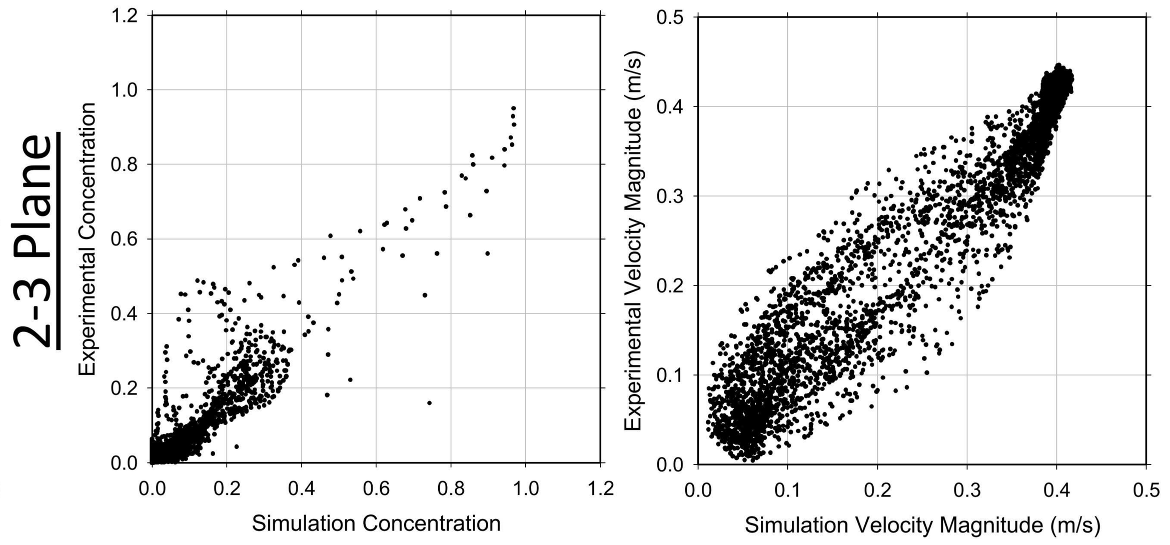
Comparisons are made on planes and volumes corresponding to planar extents including the wake of the large building. Plane images suggest good comparison between simulation and experiment.



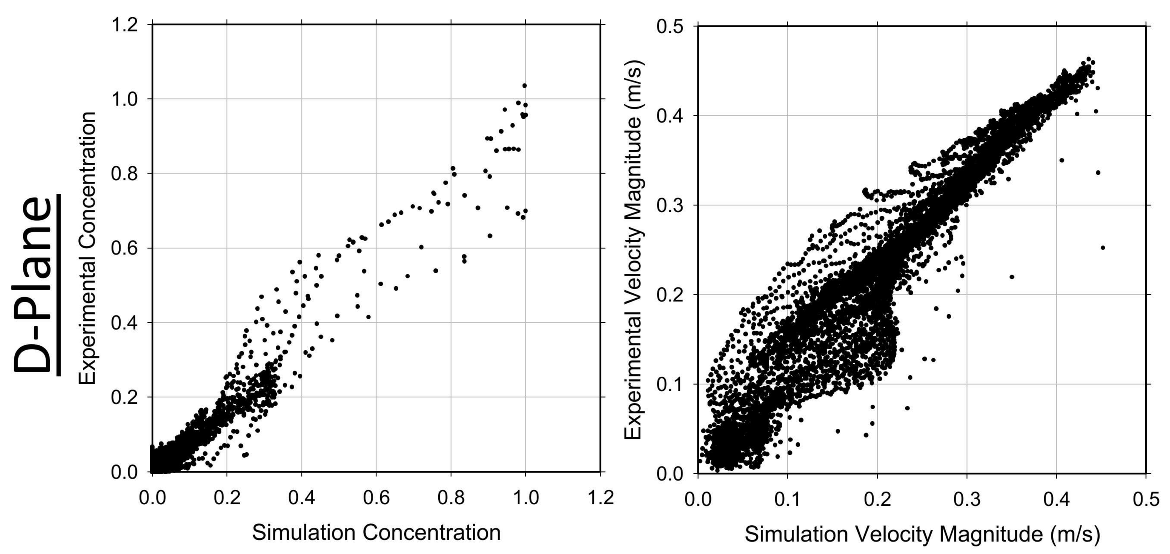
Results (continued)

Scatter plots and metric comparisons give a better comparison including quantitative measures relating to how well the data compare to the simulations on these two planes

Concentraton Velocity



Parameter	Conc.	Vel Mag.	Ideal
FB	-0.054	0.022	0
NMSE	0.272	0.022	0
MG	0.323	0.005	0
VG	11.56	1.14	0
FAC2	0.709	0.924	1
NAD	0.173	0.057	0
LND	0.404	0.169	0
LLR	0.906	0.220	0



Parameter	Conc.	Vel Mag.	Ideal
FB	0.365	0.083	0
NMSE	0.197	0.031	0
MG	0.008	0.014	0
VG	1.38	1.11	0
FAC2	0.837	0.953	1
NAD	0.137	0.073	0
LND	0.292	0.175	0
LLR	0.404	0.2175	0

It is also instructive to perform a correlation analysis on the results matrix. This analysis includes gradient variables, and besides including an additional measure of accuracy also has the potential to help identify error sources and develop hypotheses regarding simulation improvement strategies.

D-Plane

Variable	R^2	Variable	R^2
Conc.	0.930	Y-Conc. Grad.	0.662
Velocity Mag.	0.927	Z-Conc. Grad.	0.725
X-vel	0.186	Vort. Mag.	0.640
Y-vel	0.887	X-Vort.	0.560
Z-vel	0.961	Y-Vort.	0.310
Conc. Grad.	0.859	Z-Vort.	0.098
X-Conc. Grad.	0.056	Q-crit	0.295

2-3 Plane

Variable	R^2	Variable	R^2
Conc.	0.783	Y-Conc. Grad.	0.388
Velocity Mag.	0.926	Z-Conc. Grad.	0.640
X-vel	0.680	Vort. Mag.	0.721
Y-vel	0.781	X-Vort.	0.636
Z-vel	0.945	Y-Vort.	0.726
Conc. Grad.	0.702	Z-Vort.	0.399
X-Conc. Grad.	0.132	Q-crit	0.222

Summary

Comparisons are made between SIERRA/Fuego and MRC/MRV experiments for concentration and velocity. Plane images suggest good comparison between simulation and experiment. Comparison methods help quantify the accuracy of the comparison and provide benchmark accuracy for scenarios of this type. A variety of metrics are presented along with correlation based coefficients of determination.

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**Hanna, S. and Chang, J. "Acceptance criteria for urban dispersion model evaluation." Meteorology and Atmospheric Physics, 116(3-4), pp.133-146, 2012.