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

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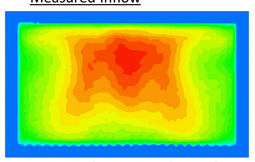
Abstract

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 fluid 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 45 degree scenario. This is similar to the scenario described in "Detailed 3D flow and concentration methods and validation with MRC/MRV techniques I" except that the mock buildings are rotated 45 degrees relative to the incoming flow. We present new techniques for comparing simulated concentration and velocity values to the MRC/MRV data. We also examine how boundary conditions and mesh effects can affect the quality of the simulation results. This work provides benchmark accuracy metrics for SIERRA/Fuego and also provides guidelines on recommended methods for subsequent comparisons of this nature.

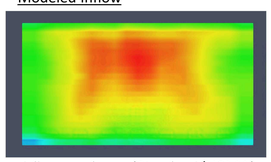
Methods

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

Measured Inflow

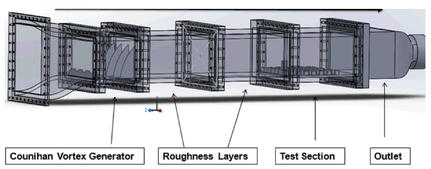


Modeled Inflow



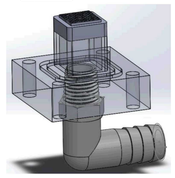
Additive manufacturing is used to construct the water channel, injectors, and flow surfaces (Stanford/USMA)

Channel



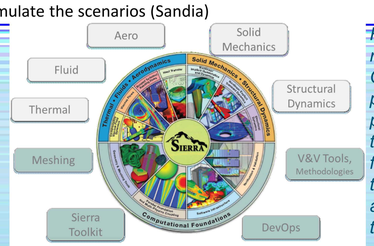
Test section

Injector

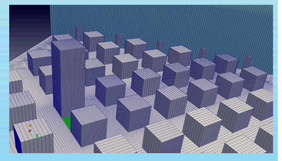


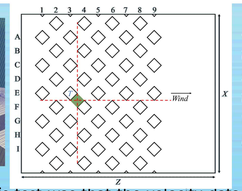
SIERRA/Fuego is used to simulate the scenarios (Sandia)

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 the locations in the domain. The square with a 'T' is the tall building, and the injector is green in both images.

A differentiating feature of this test was that the velocity data were taken with no concentration flow (plug instead of an injector) under the hope that the flow effect would be minimal. These data help identify the magnitude on quantitative outputs of a discrepancy of this nature. 3D comparisons are made for experimental concentrations > 0.025 at 197,000 point locations.

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:

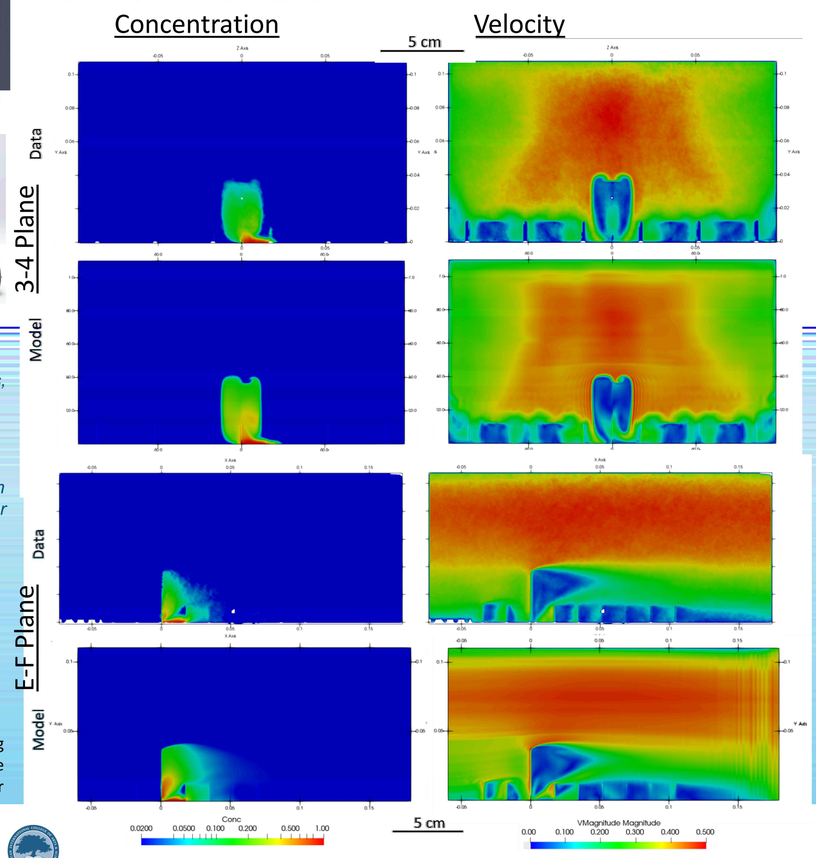
- The Fractional Mean Bias (FB): $2\left(\overline{C_o} - \overline{C_p}\right)/\left(\overline{C_o} + \overline{C_p}\right)$
- The Normalized Mean-Square Error (NMSE): $\overline{\left((C_o - C_p)^2\right)}\Big/\left(\overline{C_o} \times \overline{C_p}\right)$
- The Geometric Mean (MG): $exp\left(\overline{lnC_o}\right)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

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:

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

Results

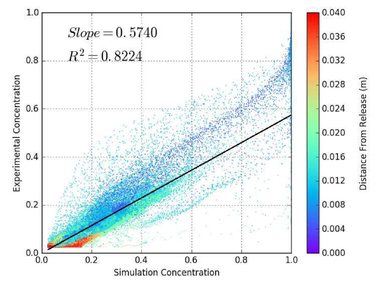
Comparisons are made on planes and volumes corresponding to planar extents including the wake of the large building. Plane images suggest good comparison between simulation and experiment.



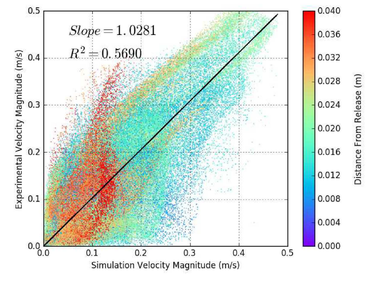
Results (continued)

Scatter plots and metric comparisons give a better comparison including quantitative measures relating to how well the data compare to the simulations for all valid concentration and velocity data points.

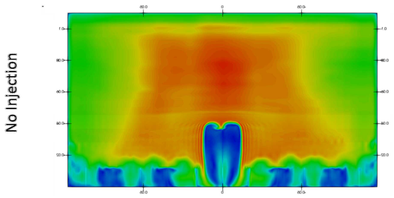
Concentration

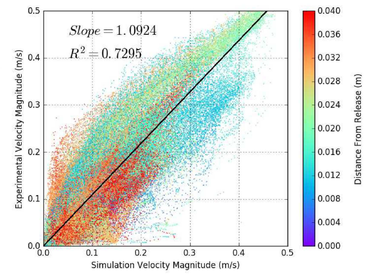


Velocity Magnitude



If a simulation is run with no injection (consistent with the way the data were taken), better agreement is found for the velocities at the 3-4 plane.





The metrics used for characterizing the accuracy of the comparisons between model and experiment are partially based on historical work and partially based on newly introduced parameters. They will be better interpreted in the context of other similar studies.

Table to the right shows quantitative metrics for the baseline simulation results and a velocity corrected simulation. Slight improvements are mostly found with improved injection flow model.

Concentration results were disappointing, and are suggestive of a general bias between simulations and experiments. Applying a bias correction, concentration results improve significantly (not shown).

Parameter	Conc.	Vel Mag.	Vel Mag. Corrected	Ideal
FB	-0.632	0.105	0.150	0
NMSE	0.386	0.192	0.129	0
MG	0.509	1.07	1.14	0
VG	1.79	1.67	1.41	0
FAC2	0.483	0.732	0.805	1
NAD	0.323	0.200	0.165	0
LND	0.456	0.355	0.309	0
LLR	0.652	0.463	0.399	0

Summary

Comparisons are made between SIERRA/Fuego and MRC/MRV experiments for concentration and velocity. Plane images suggest good comparison between simulation and experiment. Quantitative metrics comparing thousands of datapoints suggest accuracy of the model. In the context of the 3 MRC/MRV comparisons performed to date, these are the poorest. This is perhaps due to the concentration bias. These comparisons suggest the magnitude of importance the injection has on the resulting quantitative results for this test. These also set benchmark accuracy for subsequent 3D validation studies.

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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.