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Detailed Advection and Diffusion Validation of CFD with MRC/MRV 3D data

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Abstract

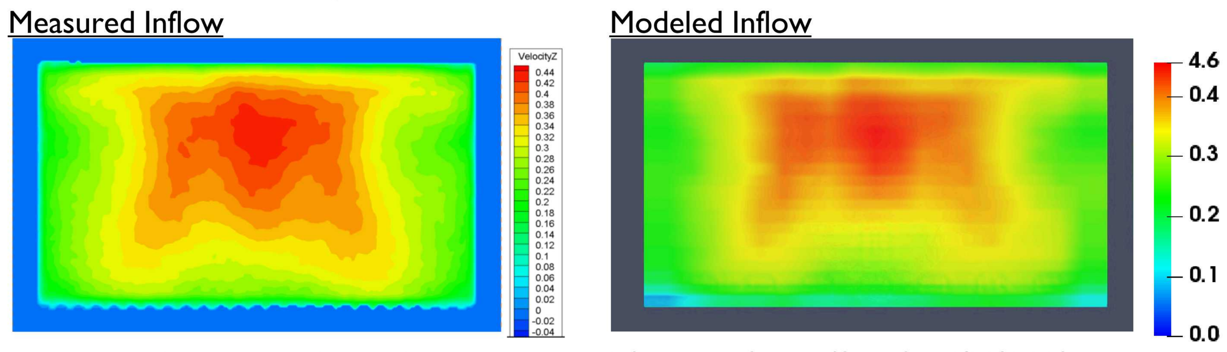
New 3D concentration and velocity vector field data are being generated using the Magnetic Resonance Concentration (MRC) and Magnetic Resonance Velocimetry (MRV) techniques. These techniques employ commercial Magnetic Resonance Imaging (MRI) instruments to measure 0.8 mm resolution 3D data in turbulent water channel flows. The detailed datasets permit spatially comprehensive comparisons to Computational Fluid Dynamics (CFD) software that simulates flow dynamics.

Three geometric datasets representative of urban geometries have been the topic of comparisons between the data and the CFD. Two scenarios are notional, and the third is designed employing 3D geometry of downtown Oklahoma City. Geometries are 3D printed for the MRC/MRV tests, and identical geometry files are used to build simulation meshes. The low-Mach number reacting flows code Fuego from the SIERRA suite of codes is used to simulate the test conditions. 2D mean inflow velocity boundary conditions are provided by the test team from the MRV measurements.

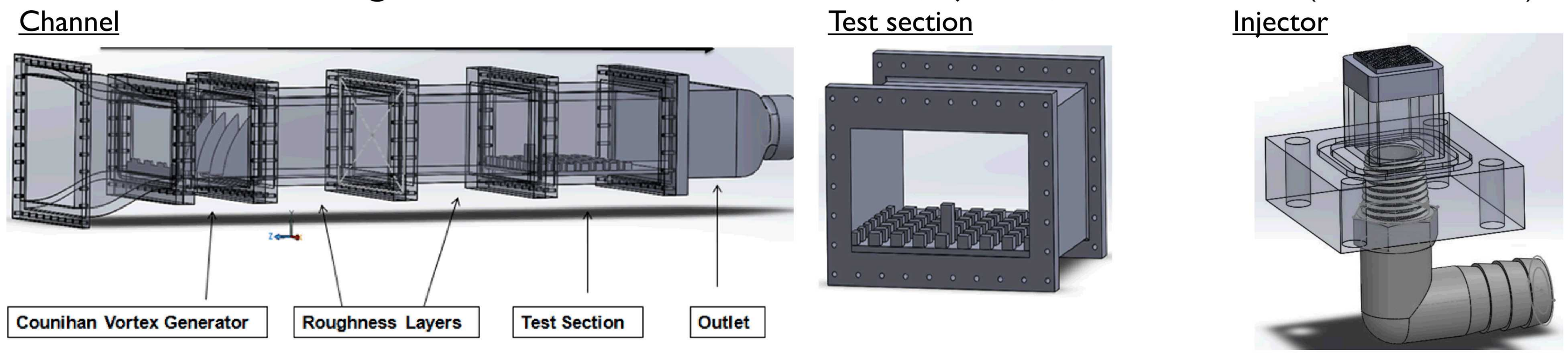
Simulation predictions are made by conducting a suite of simulations with varying parameters. The parameters are selected to be representative of input uncertainties and can thus be used to assess the model predictive uncertainty. Simulations compare very well with the experimental data. Point, line, and plane comparisons are performed. Local regions of deviation from the experimental results suggest future activities aimed at improving the quality of the validation exercise.

Methods

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

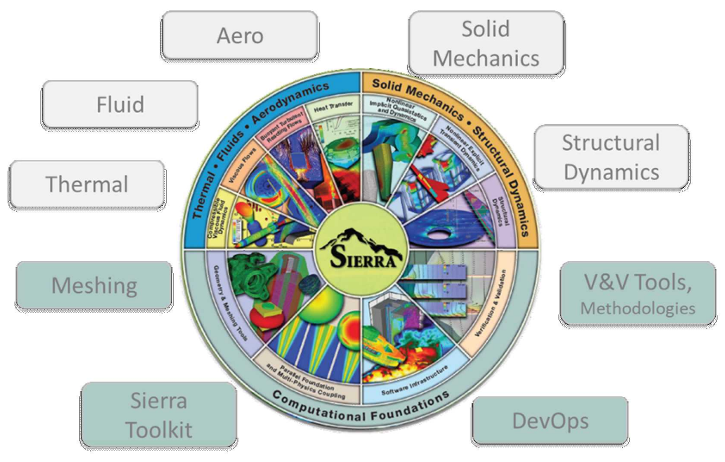


Additive manufacturing is used to construct the water channel, injectors, and flow surfaces (Stanford/USMA)



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 and Defense departments 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.

A **parameter study** such as the one shown below from the 90° scenario is used to estimate model uncertainty (Sandia)

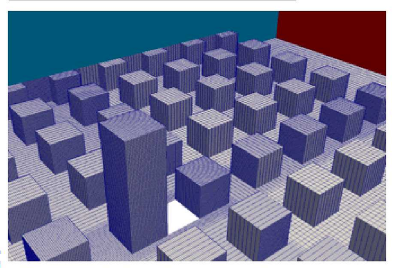
A computational matrix similar to this one is developed for each scenario to estimate model uncertainties for validation comparison purposes.

Parameter Study			
Variable:	Type	Baseline	Variation
Mesh Refinement	Numerical	Medium	Coarse, Medium, Fine
Time Step	Numerical	.0005s	+150%, +200%
Turbulence Intensity (Sub-grid)	Experimental	0%	+5%, +10%, +15%, +20%
Upwind Scheme	Numerical	Upw	upw factors, MUSCL
Residual Tolerance	Numerical	1E-5	$x10^{-1}$, $x10^{-2}$
Schmidt Number	Experimental	0.9	0.7, 0.5 (Literature Values)
Inlet Velocity Profile	Experimental	20 functions	Function accuracy, number of functions
Temperature	Experimental	21°C	±25%
Contaminant Injection Velocity	Experimental	4.4 cm/s	±10%, ±20%

Numerical parameters are used to estimate mathematical uncertainties (e.g. convergence), while experimental parameters propagate aleatoric uncertainties in model input.

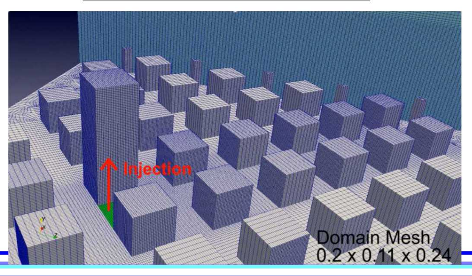
Representative results from **three scenarios** are illustrated here

90° Notional Urban



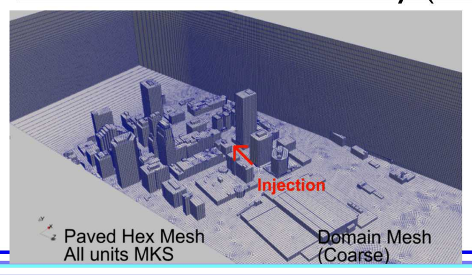
Motivated by published work based on a complex New York urban scenario with wind perpendicular to the building face.

45° Notional Urban



Same general geometry with a 45° rotation applied to the domain/wind direction. Regular array of cubic (L) buildings with a single 3L taller building

Downtown Oklahoma City (OKC)



Motivated by a test campaign that monitored gas releases in downtown OKC. This scenario 1:2500 scaled the domain based on CAD models of the city current with the dataset configuration.

Several types of classical and less traditional **validation comparisons** are enabled in this work

Point

Often validation is done comparing point data with simulation output. Selected points are used to make detailed comparisons with uncertainty on each datum.

Line

Often data and simulation lines are compared to aid in the validation process by imposing uncertainties on the outputs and expressing them as a function of distance.

Plane

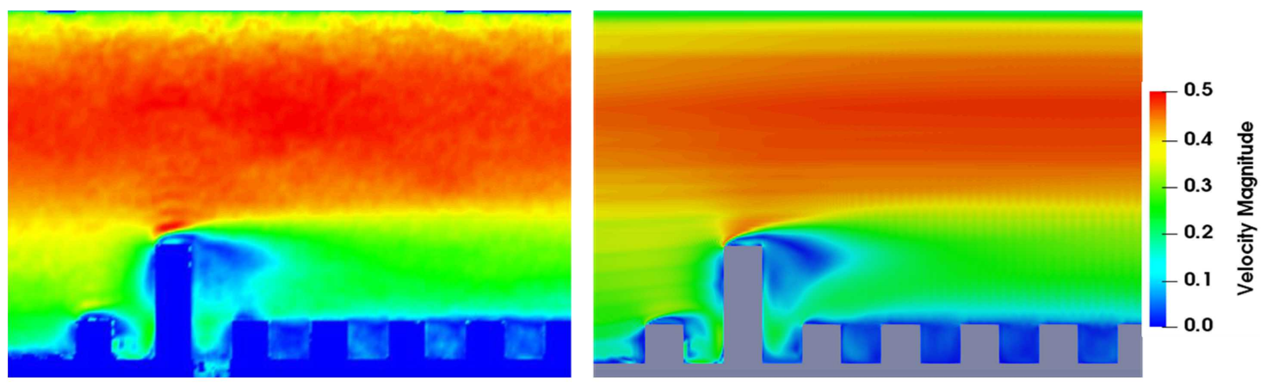
Planar data are often difficult to obtain, and make good qualitative validation comparisons through comparative contour plots. Other quantitative and statistical comparisons are also possible.

3D

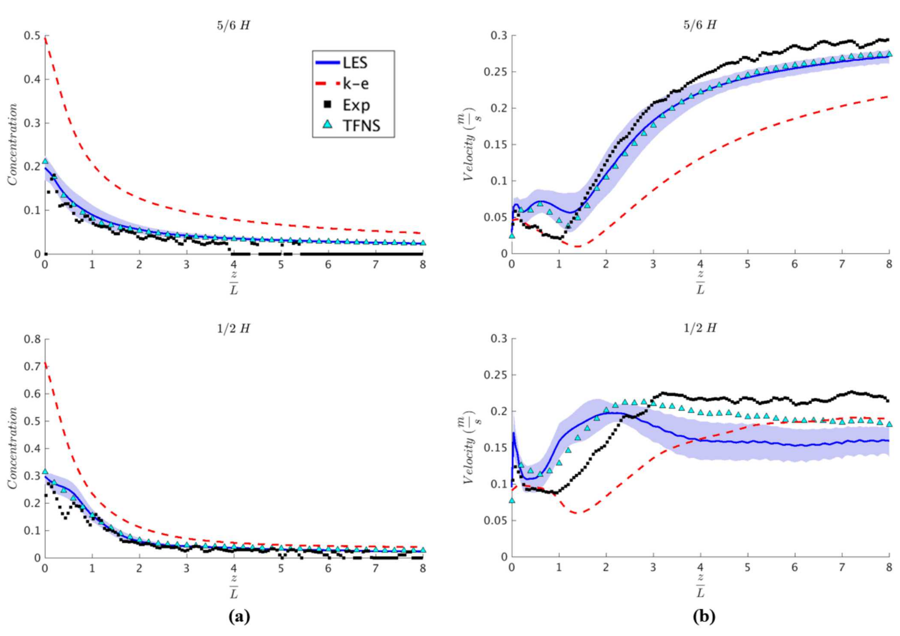
Simultaneously comparing full 3D data and models is complex, and rarely demonstrated. This is obviously ideal, but seldom do datasets exist of this nature. This is one of the prime advantages of the techniques here illustrated.

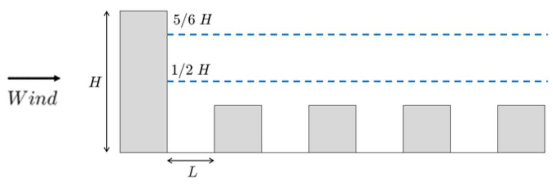
Results

The **90° scenario** produced velocities and concentrations that mostly compare well between simulation and test



Plane velocity comparisons (left) at the centerplane of the geometry

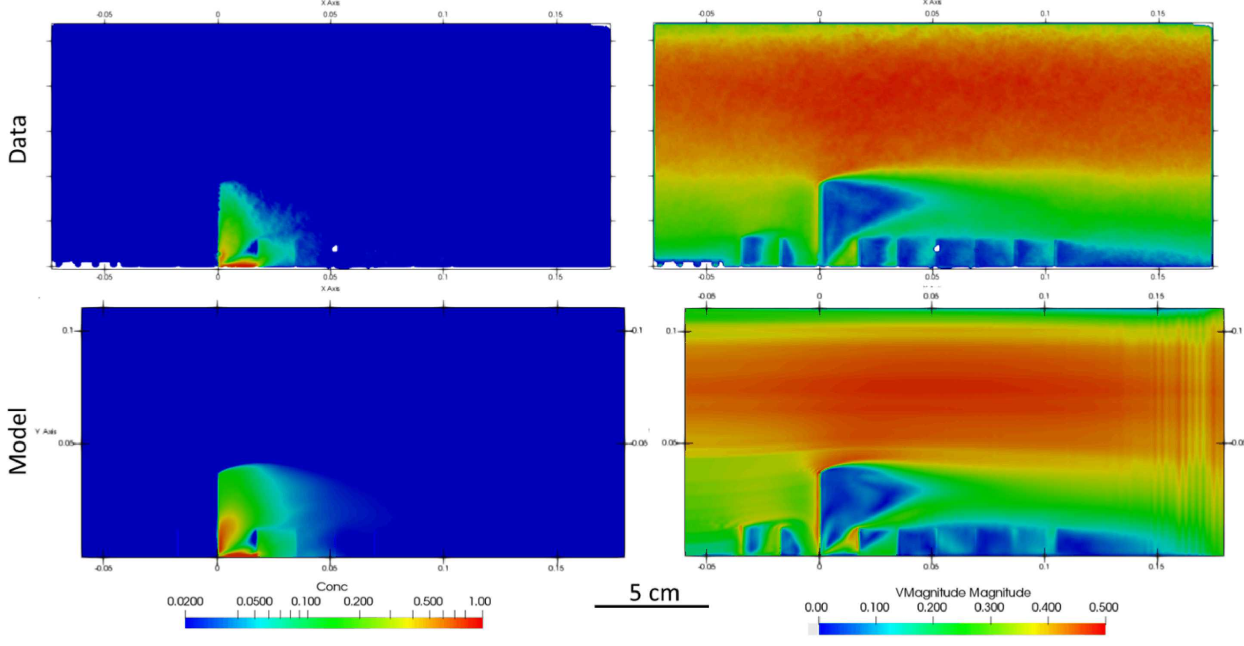


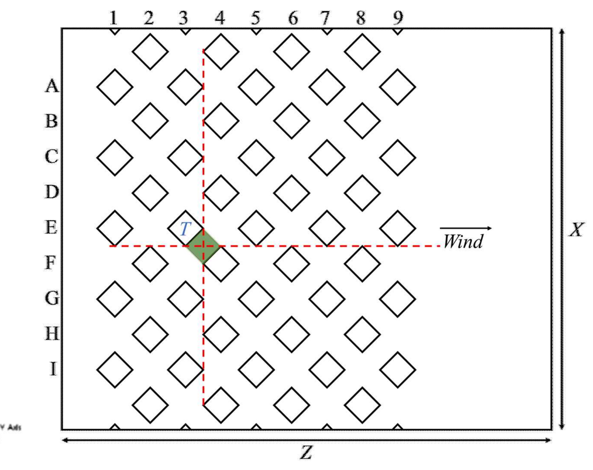


Line comparisons (left) at locations (above) and point data (below) ½ L from the downwind face of the tall building

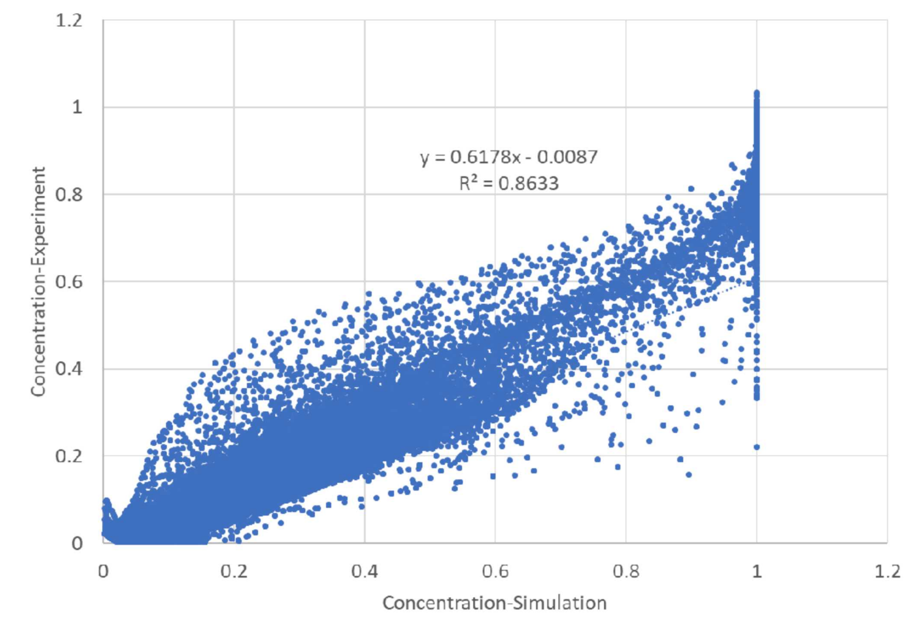
Case	Variable	5/6H μ	5/6H σ	1/2H μ	1/2H σ	1/6H μ	1/6H σ
Baseline LES	V-mag (m/s)	0.0733	0.0510	0.1077	0.0760	0.1386	0.0658
	Concentration	0.1237	0.0564	0.2562	0.1038	0.2780	0.2035
TFNS	V-mag (m/s)	0.0652	0.0474	0.1151	0.0474	0.1607	0.0695
	Concentration	0.1231	0.0470	0.2351	0.0796	0.3147	0.1545
k-ε	V-mag (m/s)	0.0334	0.0	0.0959	0.0	0.0836	0.0
	Concentration	0.3121	0.0	0.4070	0.0	0.8605	0.0
Data	V-mag (m/s)	0.0316		0.0876		0.1586	
	Concentration	0.1306		0.2507		0.2975	

The **45° scenario** results shown illustrate planar concentration and velocity magnitude as well as a 3D cloud comparison





Plane comparisons (left) at the E-F plane based on the scheme described in the top view (above)

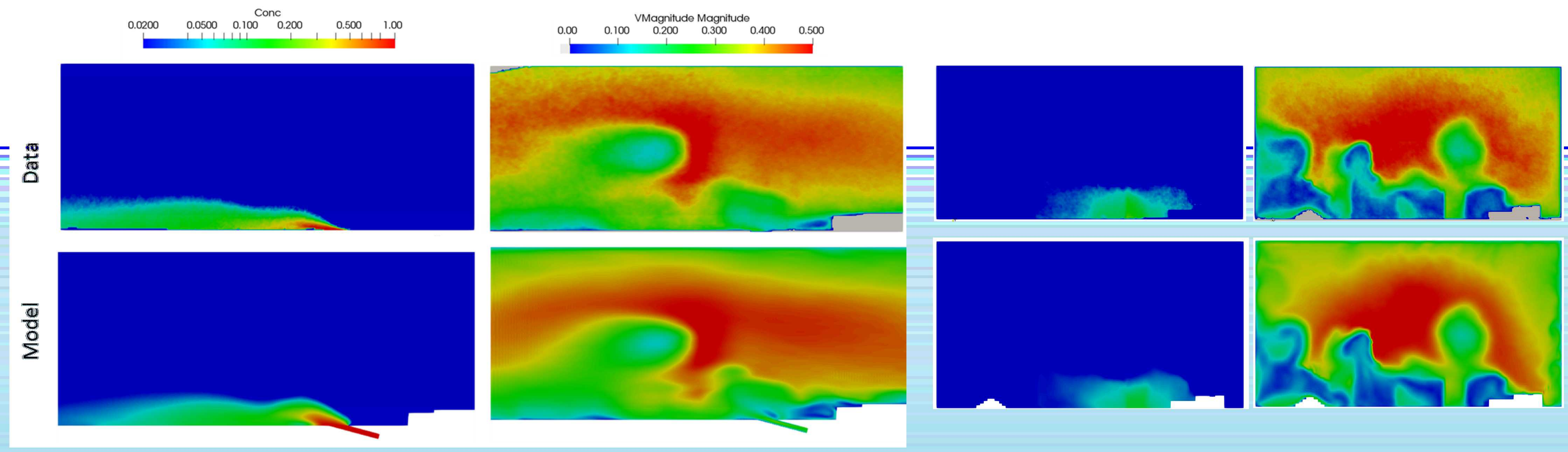


Scatter plot (left) comparisons between 4.5 x 10^5 data and simulation points shows good correlation and a bias of the prediction to a higher concentration. The model and simulation compare favorably (below), passing every metric proposed by Hanna and Chang (2012) for acceptance of plume simulation results.

H-C 2012 Criteria: FB < 0.67; NMSE < 6; FAC2 > 0.3; and NAD < 0.5

FB	NMSE	FAC2	NAD
0.651	1.167	0.472	0.325

OKC scenario results shown below illustrate selected planar comparisons at street centerplanes



Plane comparisons along Broadway Avenue (above left) and along Couch Drive (above right)

Conclusions

These techniques present a unique new opportunity for very detailed validation of turbulent flows and CFD codes. MRI instruments can provide full 3D velocity vector and concentration scalar fields in flows that are only limited by the resolution and scale of the MRI instrument and the capability of additive manufacturing to produce a flow channel that will go in the MRI. Unique and detailed validation comparisons are enabled through this work as demonstrated by example results from three predicted and tested scenarios.

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