Simulation of Turbulent Premixed Combustion

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Objective

Simulate laboratory-scale turbulent premixed combustion using detailed kinetics and transport without subgrid models for turbulence or turbulence-chemistry interaction

Premixed Low-Swirl Burner

Application:
Fundamental studies of turbulent flame dynamics

Pollutant (NO_x) formation in turbulent laboratory flame

Rod-stabilized Flame

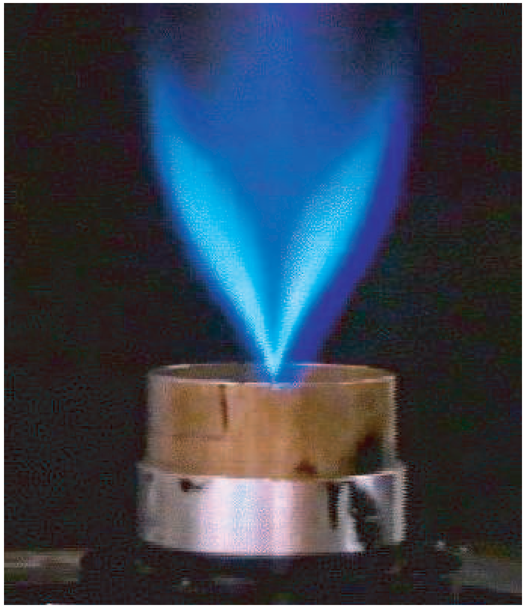


Photo courtesy R. Cheng

Traditional approach:
Compressible DNS

- High-order explicit finite-difference methods
- At least $O(10^9)$ zones
- At least $O(10^6)$ timesteps

Approach

With traditional methods, laboratory-scale simulations with detailed chemistry and transport are intractable for the near future

Observation:

- Laboratory turbulent flames are low Mach number
- Regions requiring high-resolution are localized in space

Our approach:

- Low Mach number formulation
  - Eliminate acoustic time-step restriction while retaining compressibility effects due to heat release
  - Conserve species and enthalpy
- Adaptive mesh refinement
  - Localize mesh where needed
  - Complexity from synchronization of elliptic solves
- Parallel architectures
  - Distributed memory implementation using BoxLib framework
  - Dynamic load balancing
  - Heterogeneous work load

Low Mach Number Combustion

Low Mach number model, $M = U/c \ll 1$ (Rehm & Baum 1978, Majda & Sethian 1985)

$$p(\vec{x},t) = p_0(t) + \pi(\vec{x},t) \quad \text{where} \quad \pi/p_0 \sim \mathcal{O}(M^2)$$

- p_0 does not affect local dynamics, π does not affect thermodynamics
- Acoustic waves analytically removed (or, have been "relaxed" away)
- $\vec{U}$ satisfies a divergence constraint, $\nabla \cdot \vec{U} = S$

Conservation equations:

$$\rho \frac{D\vec{U}}{Dt} + \nabla \pi = \nabla \cdot \tau$$

$$\frac{\partial \rho Y_\ell}{\partial t} + \nabla \cdot \left(\rho Y_\ell \vec{U} \right) = \nabla \cdot \vec{F}_\ell + \rho \dot{\omega}_\ell$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot \left(\rho h \vec{U} \right) = \nabla \cdot \vec{Q}$$

- Y_ℓ mass fraction
- $\vec{F}_\ell$ species diffusion, $\sum \vec{F}_\ell = 0$
- $\dot{\omega}_\ell$ species production, $\sum \dot{\omega}_\ell = 0$
- h enthalpy $h = \sum Y_\ell h_\ell(T)$
- $\vec{Q}$ heat flux
- $p = \rho R T \sum Y_\ell / W_\ell$

Fractional Step Approach

1. Advance velocity from $\vec{U}^n$ to $\vec{U}^{n+1,*}$ using explicit advection terms, semi-implicit diffusion terms, and a lagged pressure gradient.
2. Update the species, enthalpy and temperature, using explicit advection terms, semi-implicit diffusion terms, and source terms from stiff ODE integrators. Use the updated values to compute S^{n+1}
3. Decompose $\vec{U}^{n+1,*}$ to extract the component satisfying the divergence constraint.

This decomposition is achieved by solving

$$\nabla \cdot \left(\frac{1}{\rho} \nabla \phi \right) = \nabla \cdot \vec{U}^{n+1,*} - S^{n+1}$$

for ϕ, and setting

$$p^{n+1/2} = p^{n-1/2} + \phi$$

and

$$\vec{U}^{n+1} = \vec{U}^{n+1,*} - \frac{1}{\rho} \nabla \phi$$

Model problems

2-D Vortex flame interactions

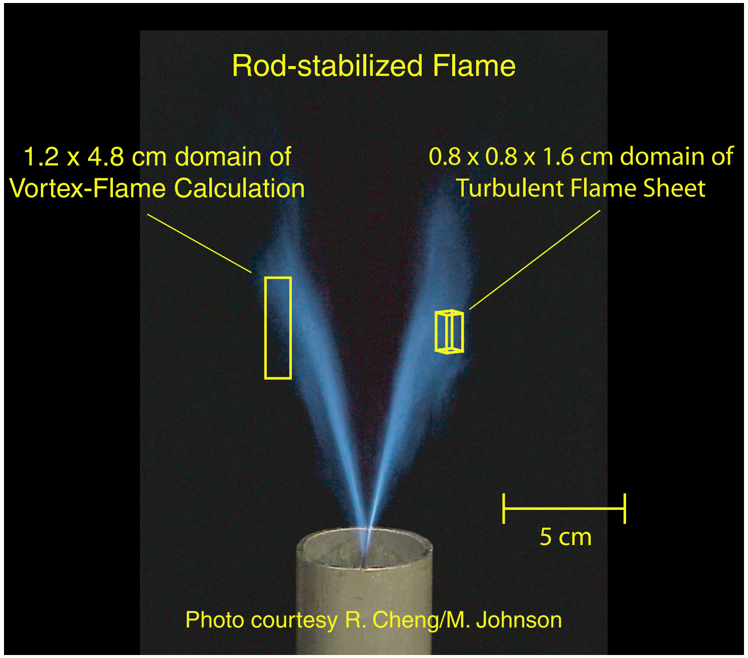
(28th International Combustion Sympsium, 2000)

- 1.2 $\times$ 4.8 mm domain
- 53 species, 325 reactions

3-D Turbulent flame sheet

(29th International Combustion Sympsium, 2002)

- .8 $\times$ .8 $\times$ 1.6 cm domain
- 21 species, 84 reactions

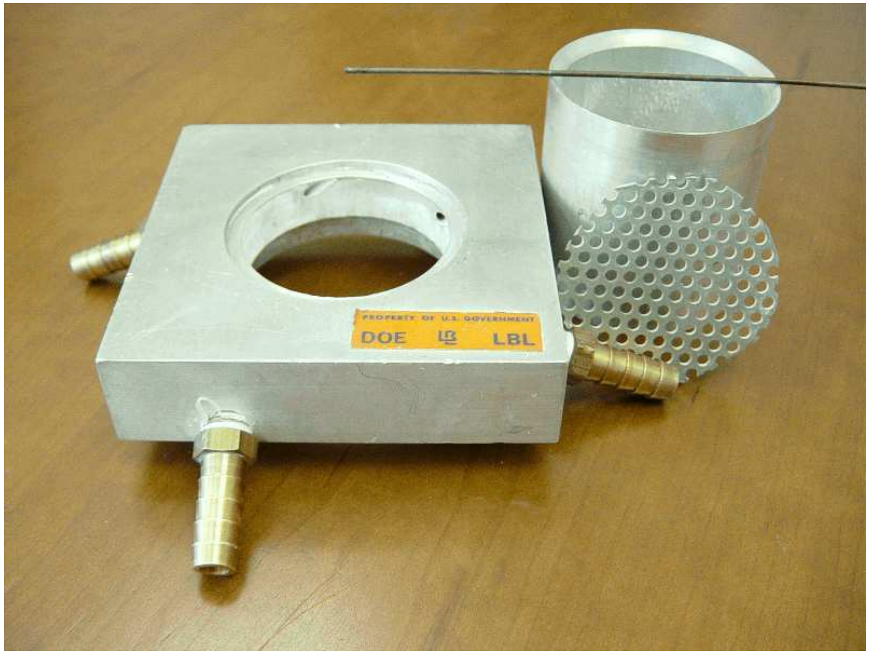


Laboratory-scale V-flame

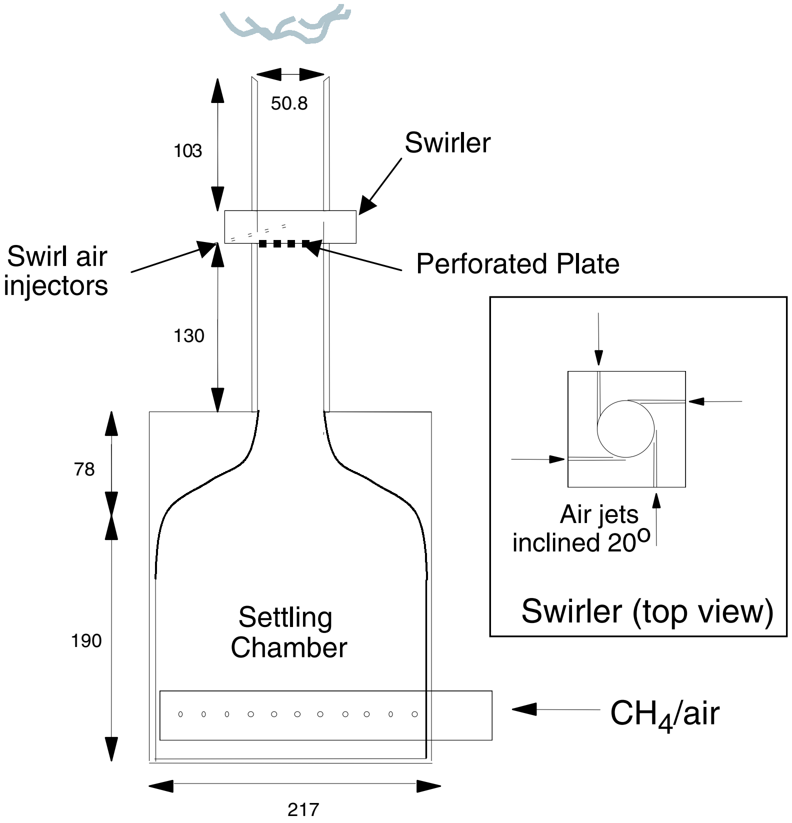
(19th International Colloquium on the Dynamics of Explosions and Reactive Systems, 2003)

- 12 $\times$ 12 $\times$ 12 cm domain
- 21 species, 84 reactions

Configuration



Burner assembly

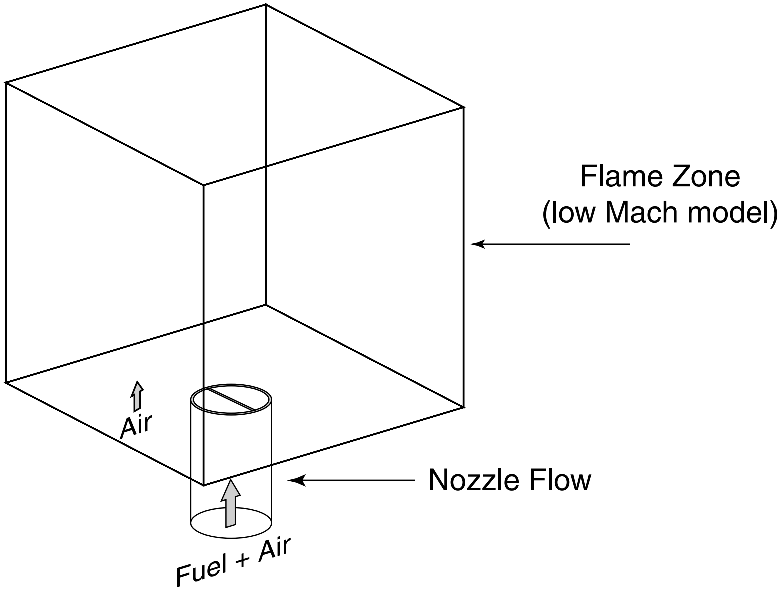


Experiment schematic

- V-flame ($\dot{m}_{air} \equiv 0$): rod $\sim$ 1 mm
- Turbulence plate: 3 mm holes on 4.8 mm center

V-flame Setup

Strategy - Treat nozzle exit as inflow boundary condition for combustion simulation



- 12cm x 12cm x 12cm domain
- DRM-19: 20 species, 84 reactions
- Mixture model for differential diffusion

Inflow characteristics

- Mean flow
  - 3 m/s mean inflow
  - Boundary layer profile at edge
  - Noflow condition to model rod
  - Weak co-flow air
- Turbulent fluctuations
  - $\ell_t = 3.5mm$, $u' = 0.18m/sec$
  - Estimated $\eta = 220\mu m$

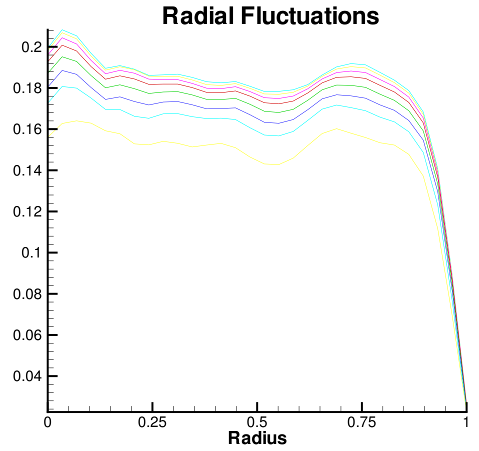
Simulate non-reacting flow in nozzle

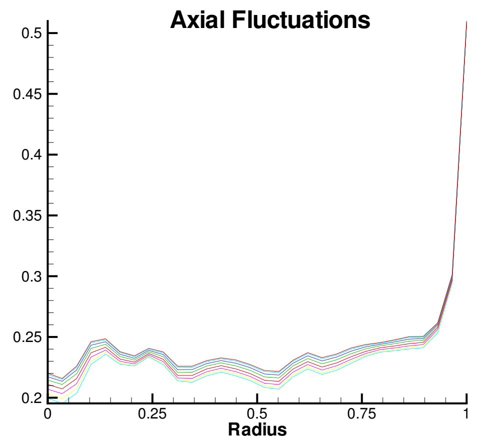
Low Mach number inflow boundary

- Direct coupling to nozzle solver
- Store nozzle outflow data
- Use statistics

Inflow turbulence

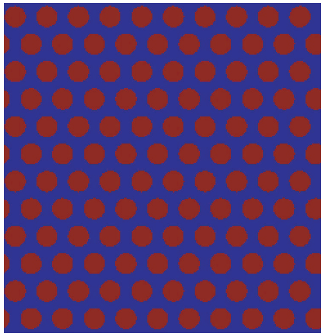
Nozzle simulation statistics



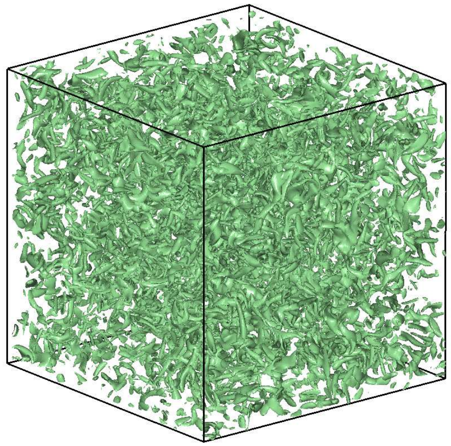


- Nearly isotropic turbulence
- Uniform except for edge effect

Initial jets



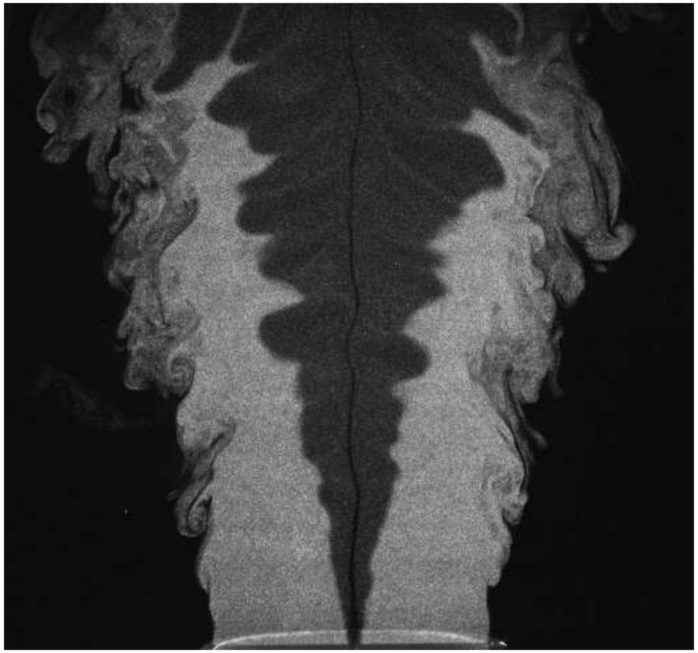
Simulated vorticity



Shape this field using statistics to prescribe turbulent fluctuations

Results: Computation vs. Experiment

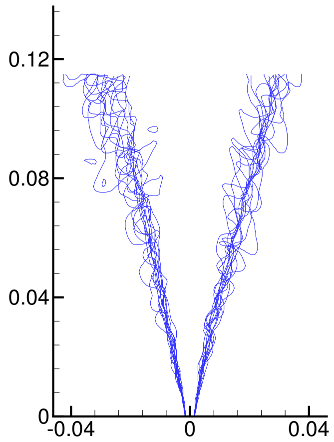
CH_4 from simulation



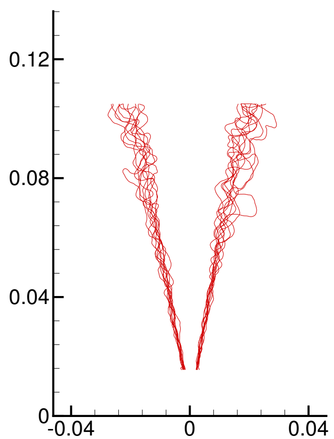
Single image from experimental PIV

Further Comparisons and Analysis

Instanteous flame surface

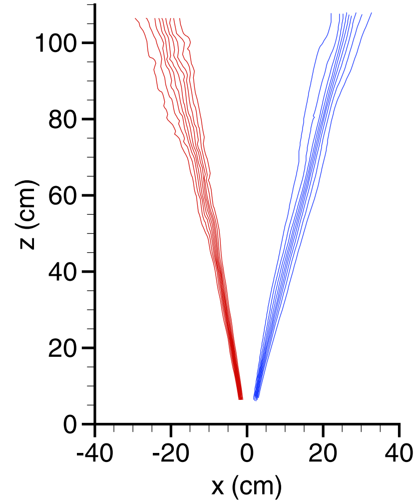


Simulation

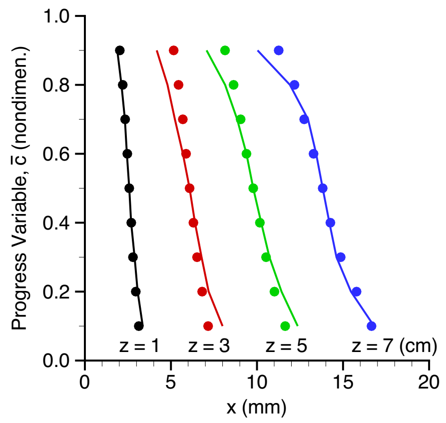


Experiment

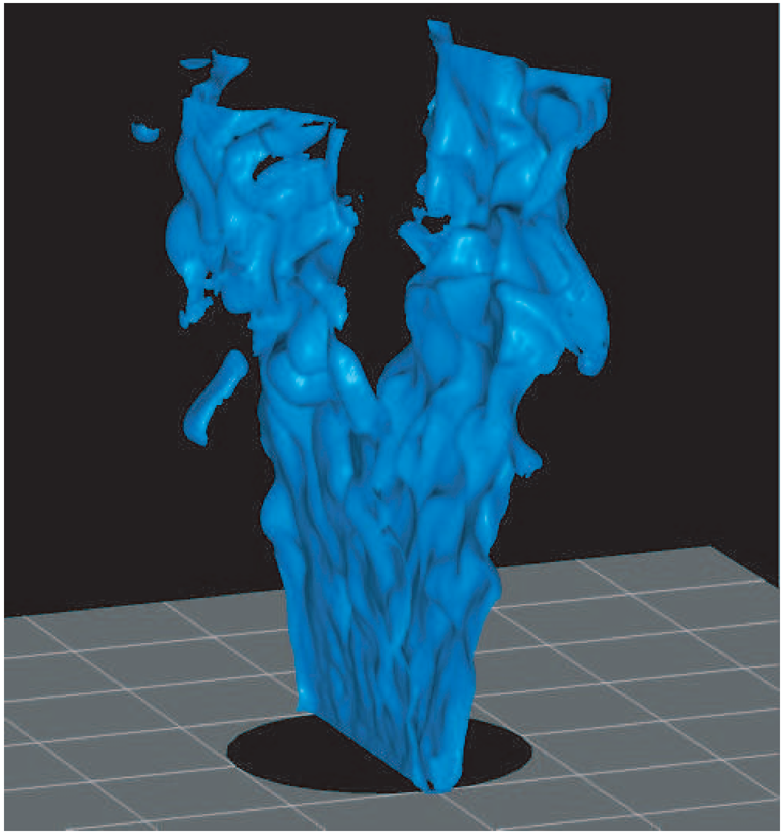
Flame brush thickness



Flame brush slices

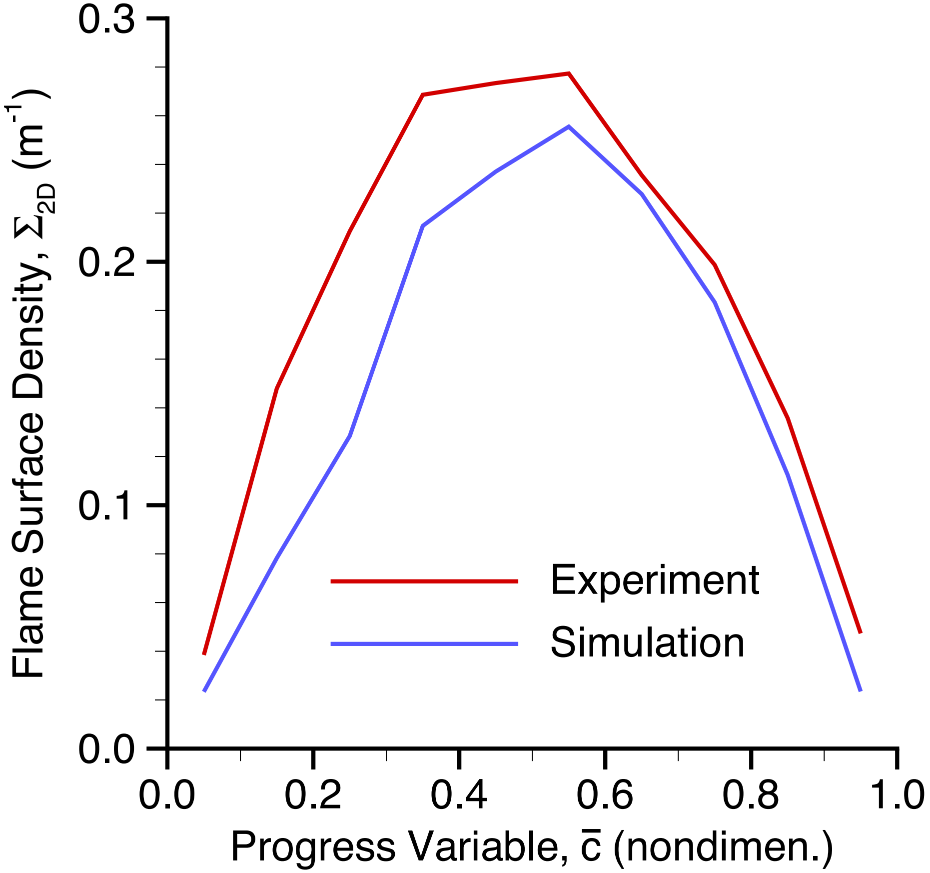


Flame Surface

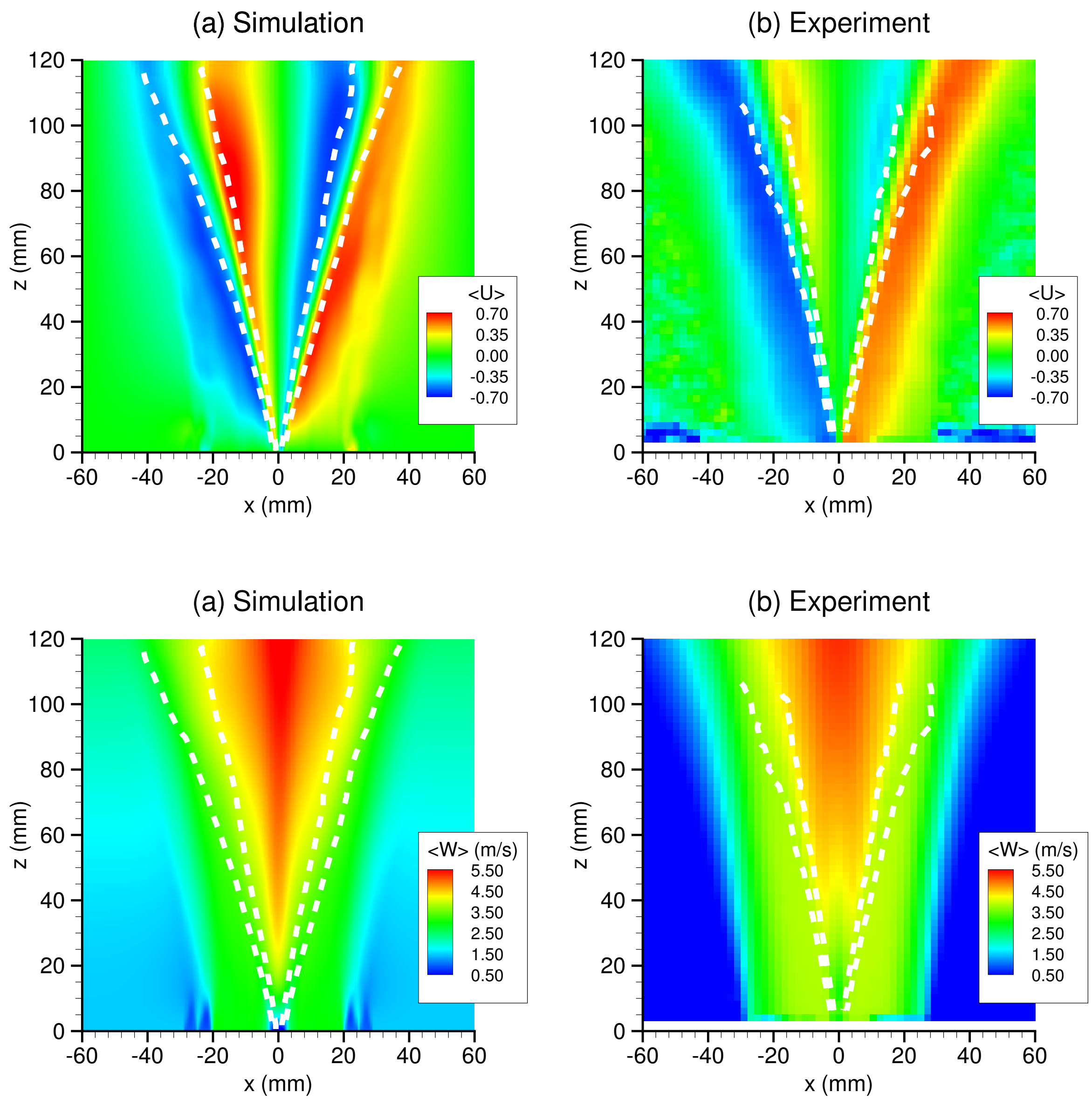


Instantaneous flame surface

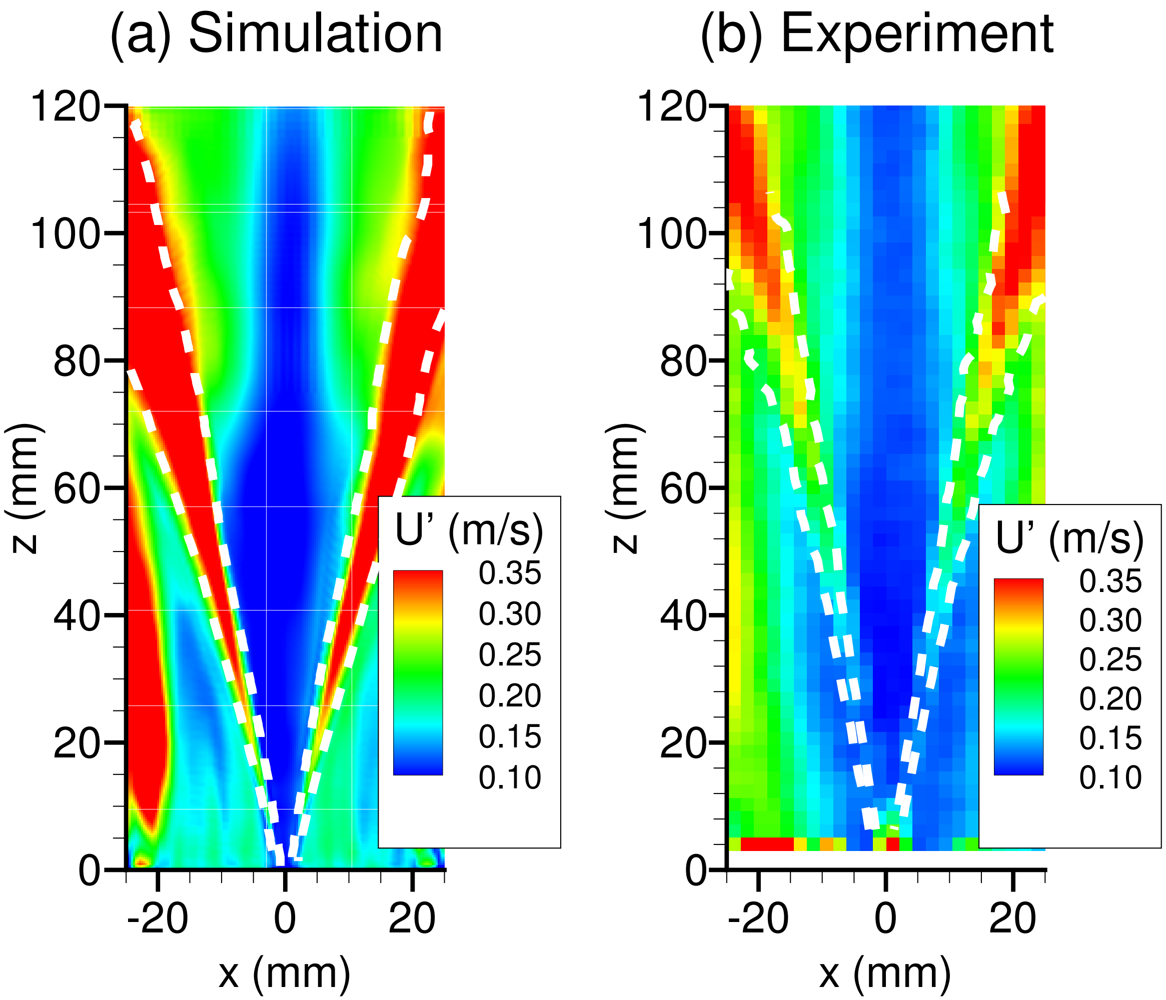
Flame surface density



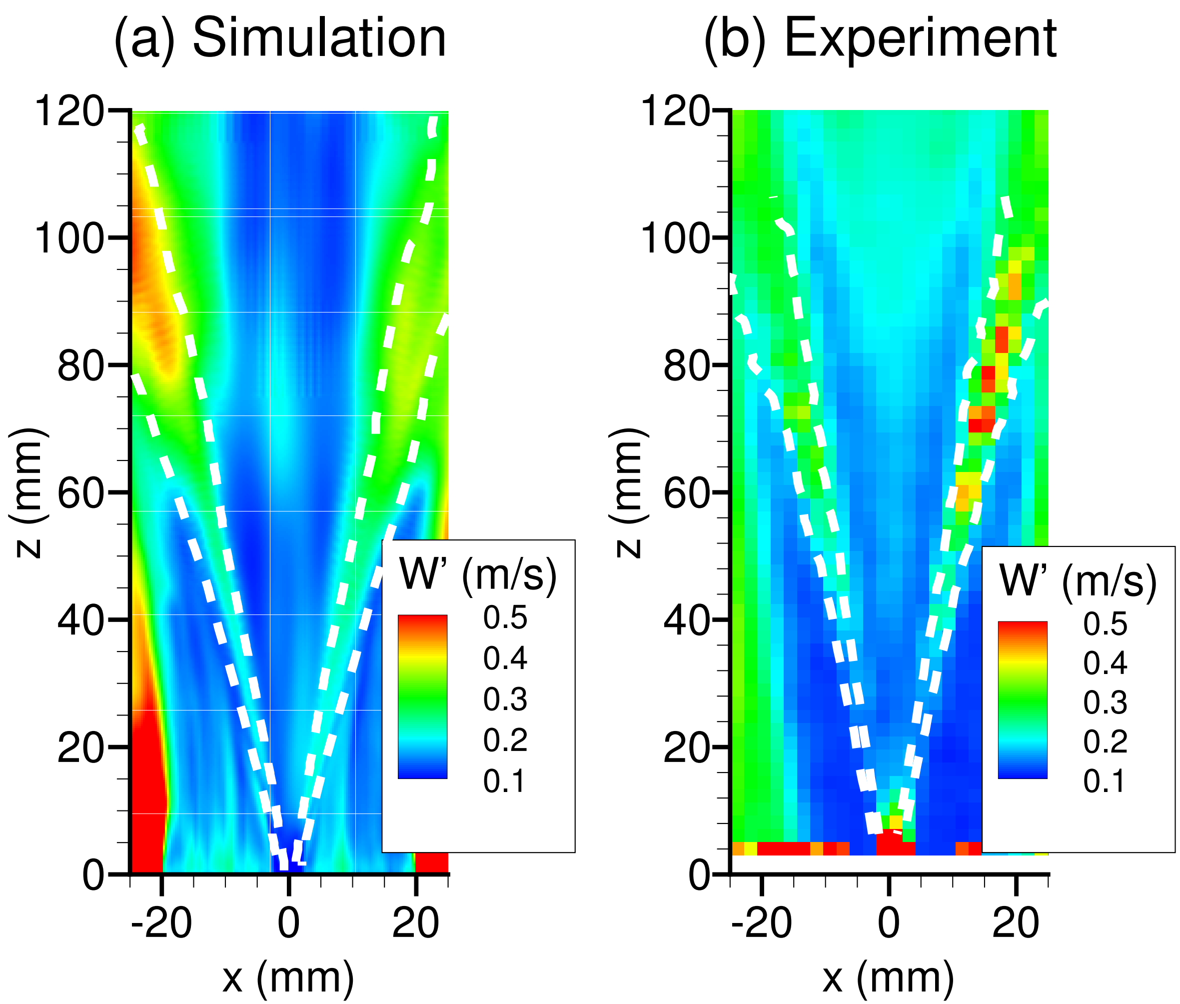
Velocity Comparisons – Means



Velocity Comparisons – Fluctuations



Velocity Comparisons – Fluctuations



Summary and Future Work

Summary

Algorithm for low Mach number combustion

- Adaptive
- Conservative
- Second-order in time and space
- Parallel

Application to laboratory-scale turbulent premixed flame

- Instantaneous flame wrinkling
- Flame brush statistics
- Velocity statistics

Future Work

- Futher validation / comparison with experiment
- Modeling of low swirl burner
- Characterize turbulent flame propagation properties
- Investigate turbulent flame chemistry