Detailed Simulations at the Laboratory Scale

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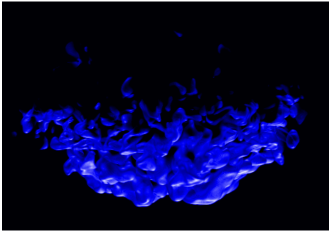

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Objective

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

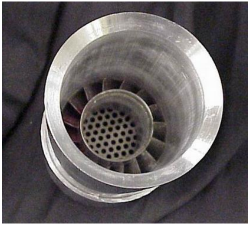
Purpose:

- Basic turbulent flame dynamics
- Model development and calibration

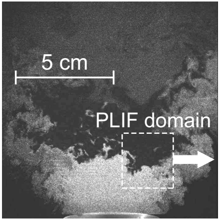
Approach:

- Conservative Low Mach formulation (Large time steps)
- Adaptive mesh refinement (Refine turbulence, flame)
- Parallel implementation (Large-scale application)

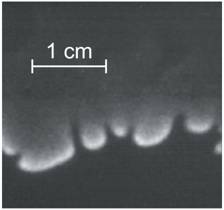
Hydrogen combustion



Mie-scattering



OH-PLIF



- OH PLIF shows gaps in the flame
- How do these flames burn?
- Are existing engineering models applicable?
- Can standard flame analysis techniques be used to analyze structure?

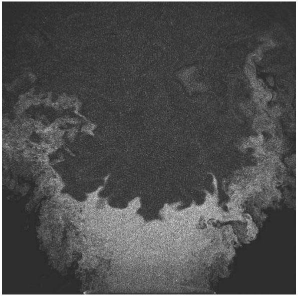
Relevant Scales

Spatial Scales

- Domain: ≈ 10 cm
- Flame thickness: $\delta_T \approx 1$ mm
- Integral scale: $\ell_t \approx 2 - 6$ mm

Velocity Scales

- Flame speed $O(10^2)$ cm/s
- Mean Flow: $O(10^3)$ cm/s
- Acoustic Speed: $O(10^5)$ cm/s



Mie Scattering Image

Fast chemical time scales but energy release coupling chemistry to fluid is on slower time scales

Sample Cases

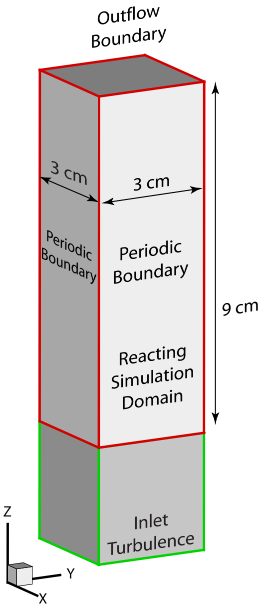
Focus on two cases:

1. Idealized “box” geometry with lab-scale dimensions
   - Show some details of the thermo-diffusive instability
   - Demonstrate existing diagnostics
2. Low swirl burner cases (brand new)
   - Show general flame shape (CH_4 vs. H_2)
   - Validate numerical convergence
   - Request help in analysis

Sample Cases

Case 1: Idealized “box” geometry with lab-scale dimensions

Computational Setup



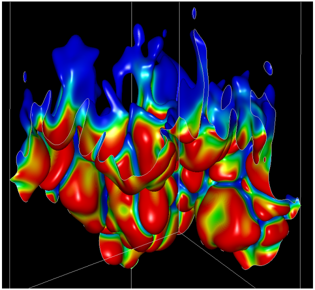
Idealized computational domain

- Approximates core region of LSB
- In/out flow + periodic domain
- Numerically controlled mean inlet flow
  - Dynamically adjusted to hold flame 2 cm above inlet
- Turbulent fluctuations added to inlet
  - $\ell_t = 3$ mm, $u' = 45$ cm/s, slightly anisotropic (LSB plate turbulence)
  - "Wrinkled laminar flamelets"

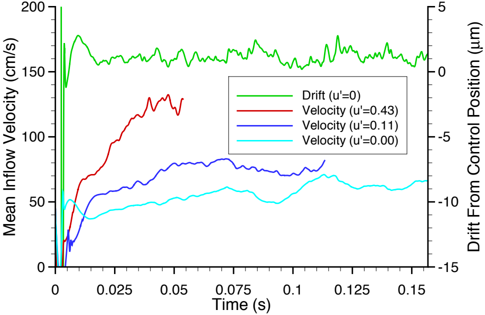
Simulation

- Detailed H_2 chemistry/transport
- $\Delta x_{eff} = 58\mu$m, AMR fine grid dynamically tracks flame surface

Simulated Lean Hydrogen Flame

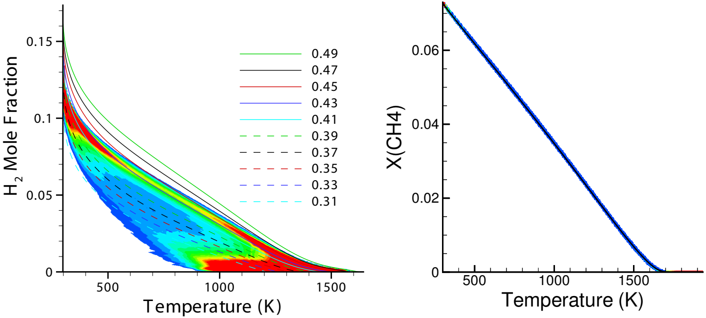


Isotherm $T = 1200$ colored with fuel mass consumption rate (blue $\rightarrow$ 0)



- $\tau = \ell_t / u' \approx$ 7 ms (strong), 27 ms (weak)
- After fast initial transient, flame position controlled smoothly and indefinitely
- Control velocity $\equiv$ turbulent burning speed, shows large variability

Chemistry in Hydrogen Flames



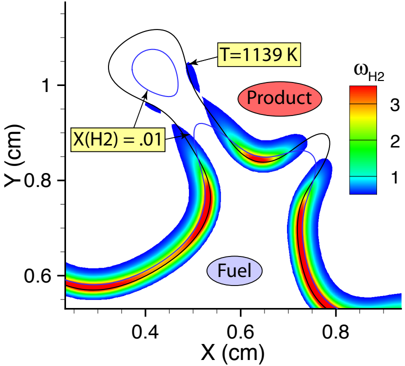
- Significant difference in burning characteristics
- Most burning occurs at conditions substantially different than laminar flame

Hydrogen flame – detailed analysis

Thermodiffusive instability complicates flame analysis

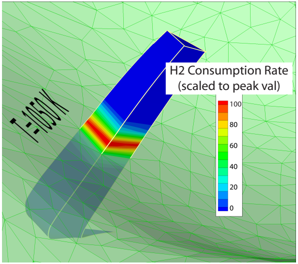
- Choice of progress variable
- Definition of the flame

Slice from 3D-simulation



Flame surface diagnostics

Discretize the flame zone based on an isosurface of the flame "progress" variable (we use T here)



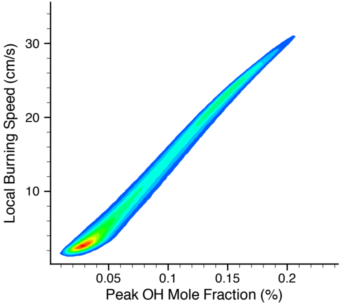
$$s_c = -\frac{1}{A_f(\rho Y_{H2})_{in}} \int_V \dot{\omega} dV$$

Local consumption speed

The normals and wedge volumes, or flame elements, can be used to characterize local flame/turbulence properties.

Characterizing Local Burning

Correlation of flame speed to OH

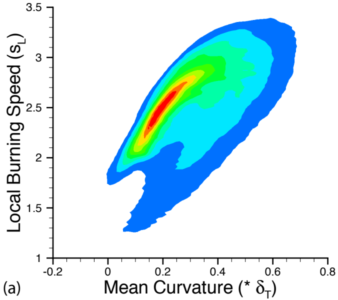


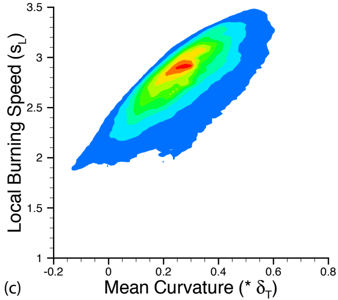
Joint PDF
(volume-weighted)

- Peak OH concentration along progress normals
- Strongly correlated distribution
- Values occur where $T = 1200 - 1300$ K
- Surface-based analysis allows us to relate downstream OH to local burning

Confirms that a quantitative measurement of local consumption speed is possible for these flames based on OH-PLIF

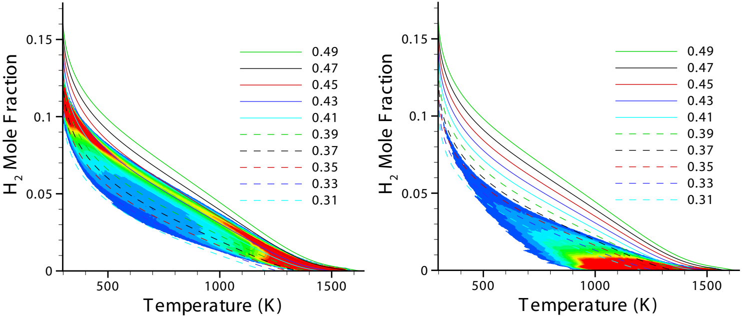
Curvature vs. Burning Speed





- Strong “Markstein” effects for no-turbulence case
- Reduced effects in strong–Le$\rightarrow$1?
- Most probable values higher, even for $\kappa = 0$, Smaller variance also?

Conditioned Hydrogen Chemistry



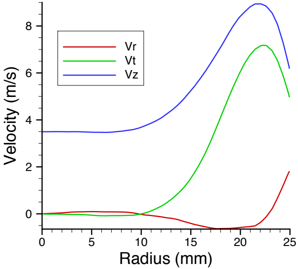
- Sort local flame elements into “burning”, “non-burning”
- Non-burning elements have no fuel in cold region
- Burning cells behave like $\phi = 0.43$ flame
- Strain rate...integrated strain, etc..

Case 2: Low swirl burner

Low Swirl Burner Simulations

Strategy:

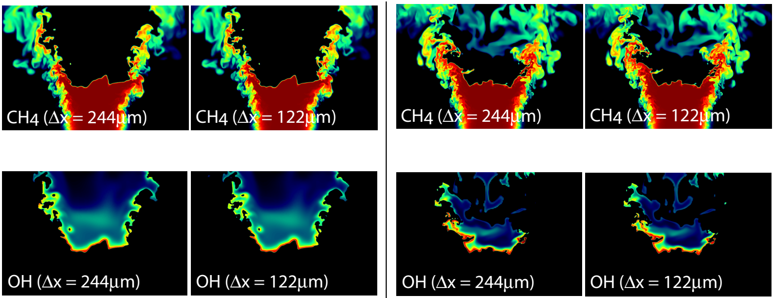
- Treat outflow from the nozzle as an inflow boundary condition
  - Mean flow and turbulent intensities from measured data
  - Impose synthetic turbulence as a perturbation to mean inflow
- Simulate flow in a rectangular domain sitting above the outflow



Four cases

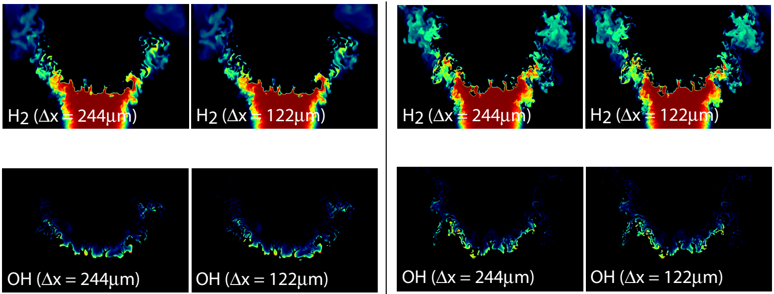
- Hydrogen ($\phi = 0.37$) and methane ($\phi = 0.7$)
- Laminar flame speed approximately 15 cm / sec
- Two levels of mean flow and turbulence

Methane swirl simulations



Weak Turbulence | Strong Turbulence

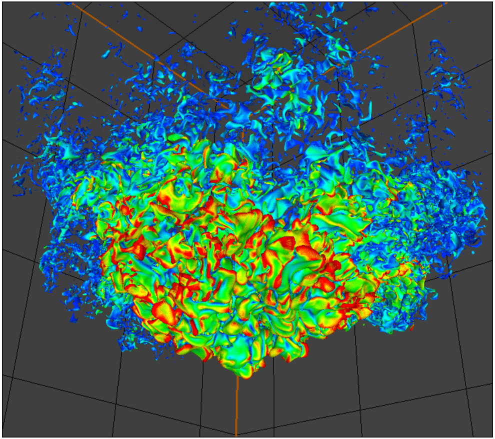
Hydrogen swirl simulations



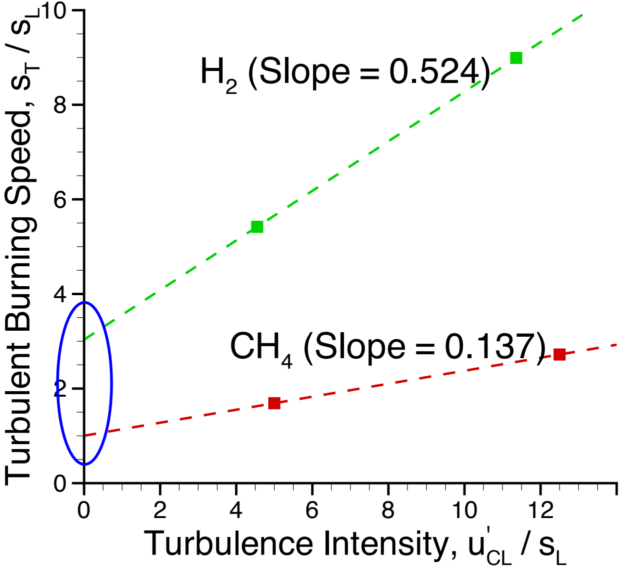
Weak Turbulence

Strong Turbulence

Hydrogen flame surface



Flame Speeds



Analysis – in progress

- Basic flame statistics
  - Flame surface: $\bar{c}$, Σ
  - Velocity: $\bar{U}$, U', ℓ_t
  - Turbulent flame properties: S_T, A_T
- Flame geometry
  - Mean and Gaussian curvature
  - Distribution of burning patches
  - Dynamics of patches – merging and splitting
- Local flame analysis
  - Local burning speed
  - Correlations with curvature, strain, etc
  - Quantify local enhancements to burning
  - Correlations to "nearby" observables on flamelet (eg, peak OH)
- Relation to experimental observables

How do all of these quantities depend on turbulence

Summary

Developed new methodology to simulate realistic turbulent flames based on exploiting mathematical structure of combustion problems

- Range of scales relevant to laboratory experiments
- Detailed chemistry and transport
- No explicit models for turbulence or turbulence / chemistry interaction
- Methodology being applied to hydrogen flames in low-swirl burner

Future work

- Closed chamber simulations
- Include nitrogen chemistry for emissions
- High-pressure simulations

Low Mach Number Formulation

Exploit natural separation of scales between fluid motion and acoustic wave propagation when mach number, $M = U/c \ll 1$ (Rehm & Baum 1978, Majda & Sethian 1985)

Start with the compressible Navier-Stokes equations for multicomponent reacting flow, expand in M. Asymptotic analysis shows that:

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

- p_0 does not affect local dynamics, π does not affect thermodynamics
- For open containers, p_0 is constant
- Pressure field is instantaneously equilibrated – removed acoustic wave propagation

Low Mach number equations

Momentum $$\rho\frac{DU}{Dt} = -\nabla\pi + \nabla\cdot\left[\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\nabla\cdot U\right)\right]$$

Species $$\frac{\partial(\rho Y_m)}{\partial t} + \nabla\cdot(\rho U Y_m) = \nabla\cdot(\rho D_m \nabla Y_m) + \dot{\omega}_m$$

Mass $$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho U) = 0$$

Energy $$\frac{\partial\rho h}{\partial t} + \nabla\cdot\left(\rho h\vec{U}\right) = \nabla\cdot(\lambda\nabla T) + \sum_m \nabla\cdot(\rho h_m D_m \nabla Y_m)$$

EOS $$p_0 = \rho\mathcal{R}T\sum_m \frac{Y_m}{W_m}$$

System contains four evolution equations for U, Y_m, ρ, h, with a constraint given by the EOS.

Constraint for reacting flows

Low Mach number system is a system of PDE's evolving subject to a constraint; differential algebraic equation (DAE) with index 3

Differentiate constraint to reduce index

$$\nabla \cdot U = \frac{1}{\rho c_p T}\left(\nabla \cdot (\lambda \nabla T) + \sum_m \rho D_m \nabla Y_m \cdot \nabla h_m\right) + \frac{1}{\rho}\sum_m \frac{W}{W_m}\nabla(D_m \rho \nabla Y_m) + \frac{1}{\rho}\sum_m \left(\frac{W}{W_m} - \frac{h_m(T)}{c_p T}\right)\dot{\omega}_m$$

Generalized projection method framework

- Finite amplitude density variation
- Inhomogeneous constraint
- Requires solution of variable coefficient, self-adjoint elliptic PDE

Low Mach number algorithm

Fractional step scheme

- Advance velocity and thermodynamic variables
  - Advection
  - Diffusion
  - Stiff reactions
- Project solution back onto constraint

Stiff kinetics relative to fluid dynamical time scales

$$\frac{\partial(\rho Y_m)}{\partial t} + \nabla \cdot (\rho U Y_m) = \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho U h) = \nabla \cdot (\lambda \nabla T) + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m)$$

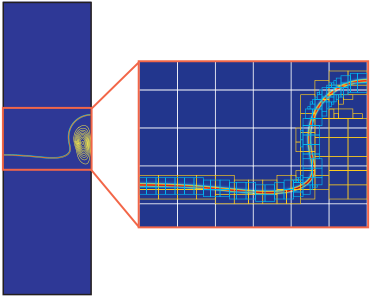
Operator split approach

- Chemistry $\Rightarrow \Delta t/2$
- Advection – Diffusion $\Rightarrow \Delta t$
- Chemistry $\Rightarrow \Delta t/2$

Block-structured AMR

AMR – exploit varying resolution requirements in space and time
Each grid patch (2D or 3D)

- Logically structured, rectangular
- Refined in space and time by evenly dividing coarse grid cells
- Dynamically created/destroyed
- Irregular work easily amortized



2D adaptive grid hierarchy

Subcycling:

- Advance level ℓ, then
  - Advance level $\ell + 1$
    level ℓ supplies boundary data
  - Synchronize levels ℓ and $\ell + 1$