Tools for Simulating Turbulent Premixed Laboratory-Scale Flames

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Presented at: SciDAC 2005
San Francisco, CA
June 26-30, 2005

Talk Outline

1. Flame theory, simulation (scales, methods)
2. Validation (sources of error)
3. Novel simulation approach (controlled flames)

Collaborators

CCSE - Internal

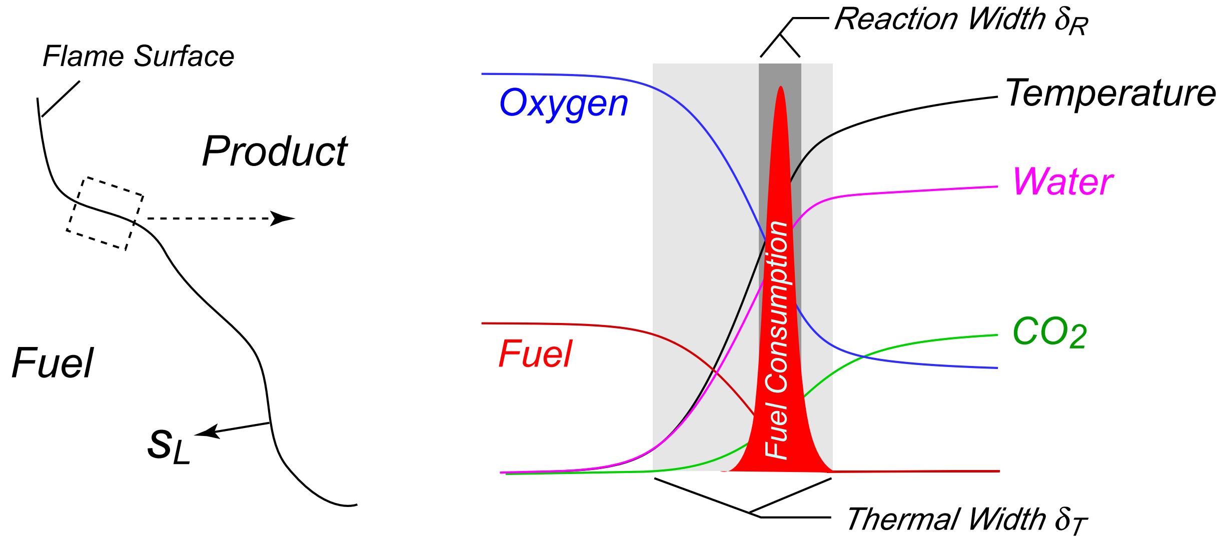
- A. Almgren
- V. Beckner
- J. Bell
- J. Grcar
- M. Lijewski
- C. Rendleman

External

- R. Cheng, I. Shepherd, M. Johnson(LBNL) - Premixed flame experiments
- S. Woosley, M. Zingale (UCSC) - Type 1a supernovae
- J. van Oijen (TU/e The Netherlands) - Generalized flamelets
- P. Glarborg, A. Jensen (DTU Denmark) - Combustion chemistry
- C. Schulz, W. Bessler (U. Heidelberg) - Flame diagnostics
- W. Green, M. Singer (MIT) - PDF method validation
- S. Tonse (LBNL) - Combustion chemistry
- C. Rutland (UW Madison) - Turbulent flame interaction, sprays diagnostics

Premixed Flames

Unlike diffusion flames, where burning rate is controlled by mixing of fuel/oxidizer, premixed flames burn freely into fuel

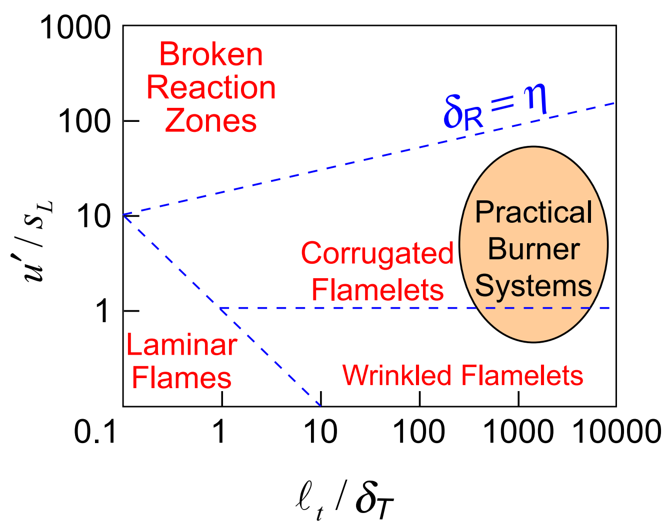


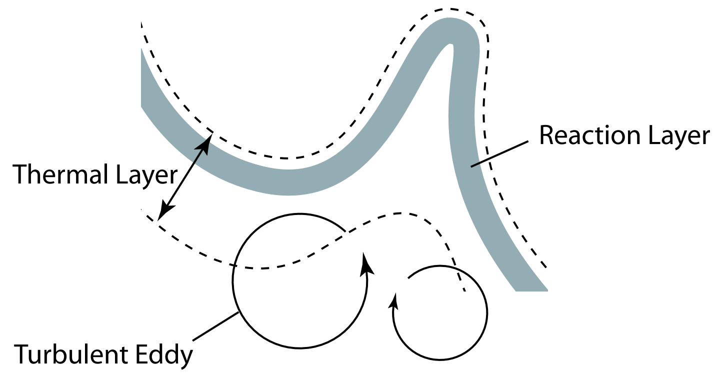
Practical considerations

- Turbulence - enhance flame surface density (efficiency/device size)
- Lean Fuel - low temperature/emissions, flame stabilization difficult

Turbulent Premixed Flames

Turbulence (ℓ_t, u') vs. flame scales (δ_T, s_L)



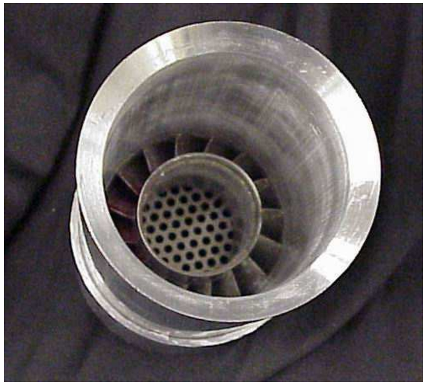
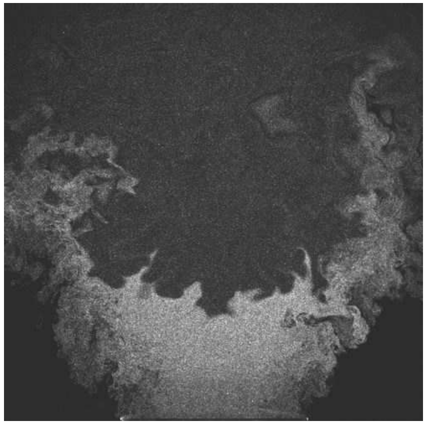


"Corrugated Flamelet"

Simulation Goal:

1. Energetics (detailed flame dynamics, stability)
2. Flame chemistry (emissions, pollutant formation)

Relevant Scales

Length and velocity scales:

- Fuel pipe: $5 - 10$ (cm)
- Flame thickness: $\delta_T \sim 600$ (μm)
- Turbulence intensity: $3 - 6$ % mean flow
- Turbulence scales: $\eta/\ell_t \sim 0.2/3$ (mm)
- Mean Flow/Acoustic Speed: $3/350$ (m/s)

"Fully-resolved" simulations require more than
$\mathcal{O}(10)$species $\times$ $\mathcal{O}(10^{12})$cells $\times$ $\mathcal{O}(10^8)$steps

Simulation Approach

Key observations

- Flow velocity $\ll$ acoustic speed
- Flame thickness $\ll$ domain size

Approach

- Low Mach number formulation
  - Remove acoustics analytically
  - No explicit models for turbulence or turbulence/chemistry interaction ("MILES" - Monotone Implicit LES)
- Adaptive mesh refinement
  - Dynamically localize computational work
- Parallel implementation
  - Distributed memory, heterogeneous load balance

Dominant costs

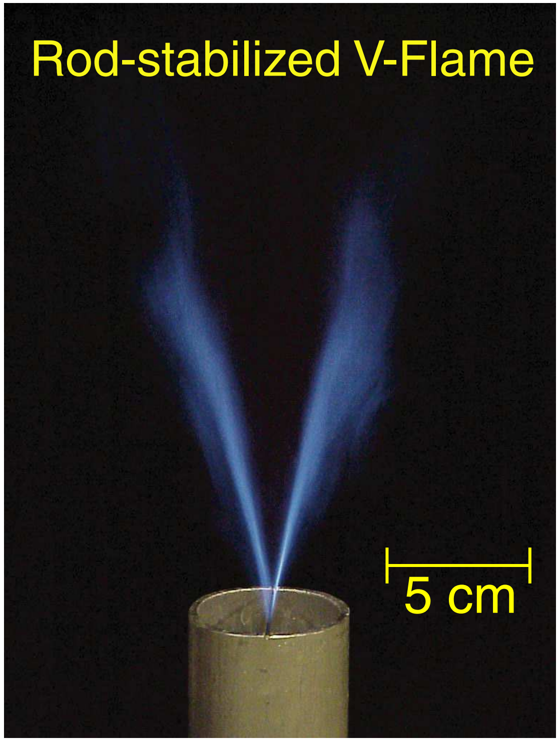
- Algorithm complexity
- Parallel communication (elliptic projection operator)
- Detailed chemistry evolution (ODE integration)

V-Flame Simulation

Strategy: Independently characterize turbulence generation in nozzle, and specify as inlet boundary conditions to reacting flow simulation

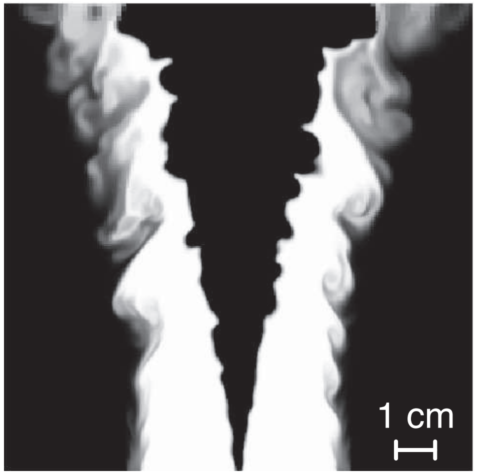
Simulation:

- $12 \times 12 \times 12$ cm domain
- Methane/air ($\phi = 0.7$) at 3 m/s
- Turbulence:
  - $\ell_t = 3.5$ mm, $u' = 0.18$ m/s (6%)
  - $\eta = 220\ \mu$m ($\Delta x = 312.5\mu$m)
- No flow condition to model rod
- DRM 19, 20 species, 84 reactions
- Differential species diffusion
- Weak air co-flow

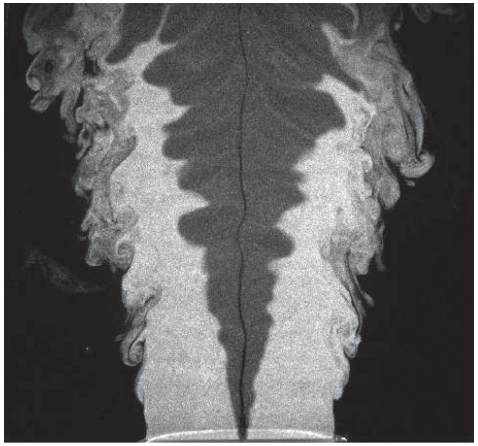


V-Flame: Validation

Simulation



Experiment



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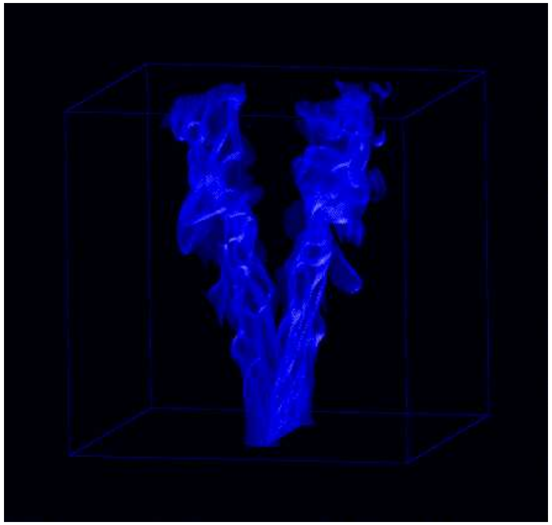
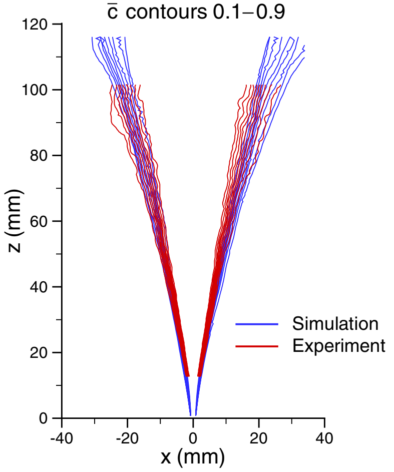
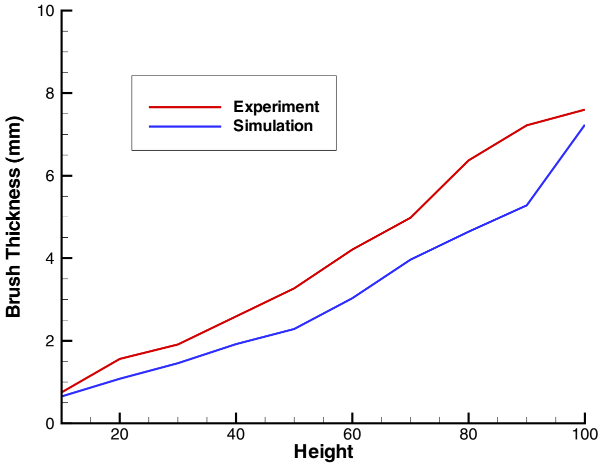
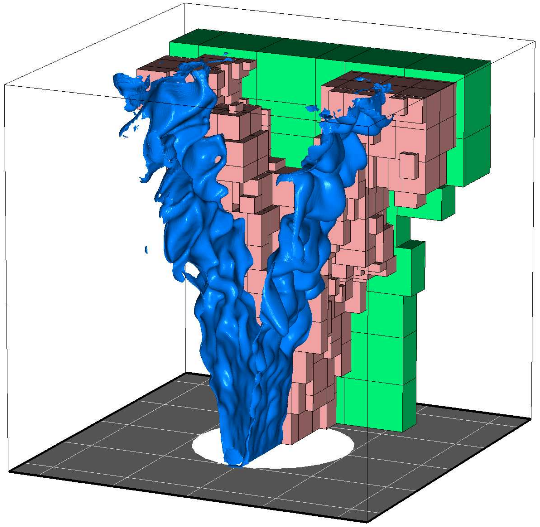








Joint work with R. Cheng, I. Shepherd and M. Johnson (to appear in PNAS, 2005).

Sources of Error

- Model assumptions, discretization errors
  - Self-consistency checks, numerical convergence analysis, etc
- Input databases, interpretation of experimental data
  - Chemical kinetics, thermodynamics, species transport
  - Data extraction from experimental observation: line-of-sight, plane-projected 3D fields, signal modification (PLIF quenching), etc.

  ....both only recently addressable for lab-scale turbulent flames

- Configuration: inlet turbulence characterization, the “laboratory response” of an unconfined flame, stabilization details
  - Can we explore flame details in a “cleaner” setting, yet remain relevant to experiments?

Controlled Premixed Flames

How does one study premixed turbulent flames?

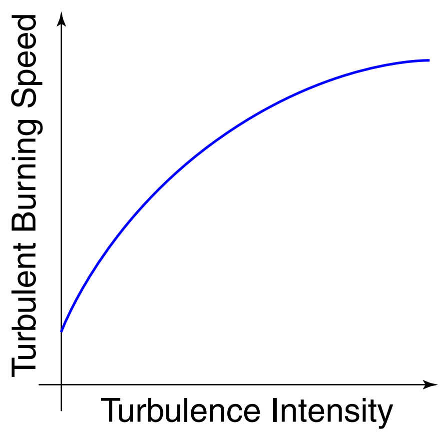
- Laboratory (requires stabilization mechanism)
  - Swirl
  - Stagnation plate
  - Rod or bluff body
  - Pilot flame or heated wire

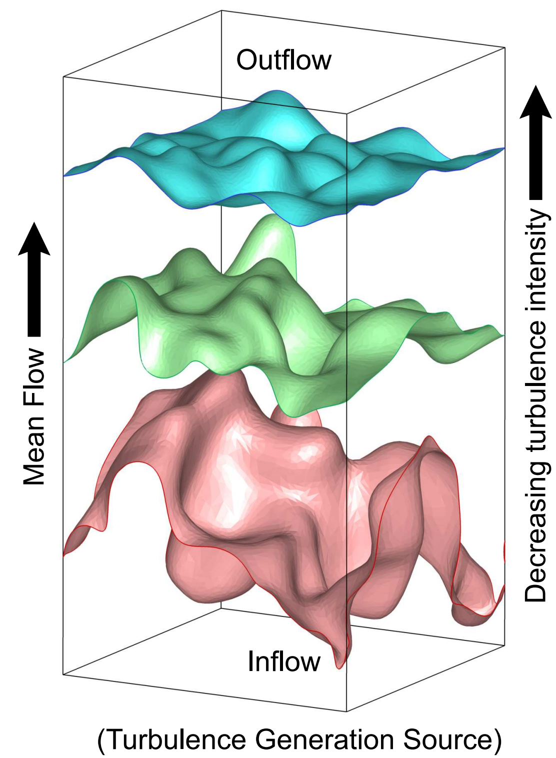
- What about computational studies?
  - Simulate a complete laboratory flame (expensive!)
  - Embed a flame in turbulence, then evolve
  - Inflow turbulence and let it interact with the flame

Rutland/Trouve (1993)
Zhang/Rutland (1995)
Bell et al. (2002)
Chakraborty/Cant (2004)
Trouve/Poinsot (1994)
Tanahashi, et al (2000,2002)
Cant et al. (2002)

Turbulent Flame Dynamics

In flamelet regimes (wrinkled, corrugated), the fuel consumption rate determined primarily by flame surface area, increases with turbulence





Propagation in spatially decaying turbulence

- Inflow too fast, flame drifts up, wrinkles less
- Inflow too slow, drifts down, wrinkles more

As in the physical situation, natural flame instability makes this configuration non-stationary.

Controlled Flame

- Use control algorithm to stabilize flame
  - Simple geometry
  - Statistically stationary
  - Detailed characterization of turbulent flame behavior
- Dynamically adjust inflow velocity, v_{in}
  - Flame location defined as total fuel mass in domain
  - Unknown turbulent flame speed, s, represents average speed of propagation
- Stochastic ODE model

$$dx = (v_{in} - s(x))\, dt + d\omega$$

  - Given $x(0)$, compute v_{in} to drive $x(t)$ to a desired value and hold it there long enough to collect flame statistics
  - Require for numerics that v_{in} be smooth and positive

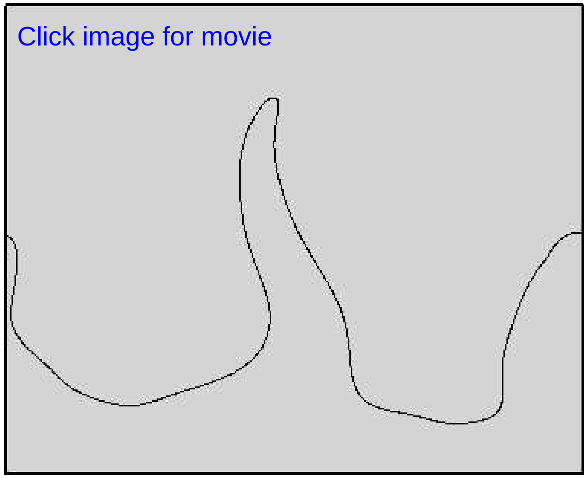
Turbulent Flame Regimes

Since (δ_T, s_L) vary with ϕ, we compute 3 controlled 2D CH_4/air flames:

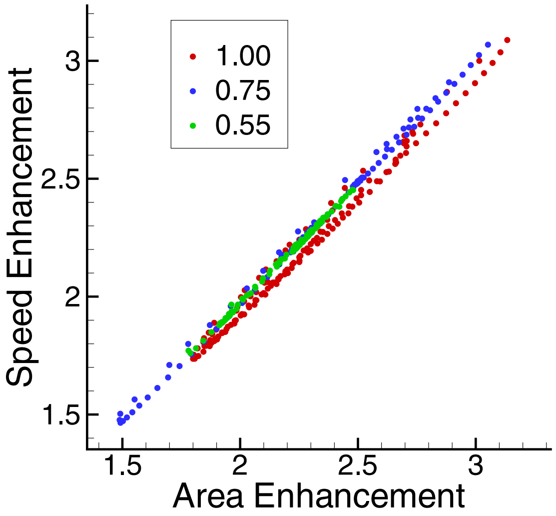
- $\phi = 0.55, 0.75, 1.0$
- GRIMech-3.0
  (53 species, 325 reactions)
- Identical scaled ℓ_t, u'
- $\Delta x = L/1024 \sim \delta_T/22$

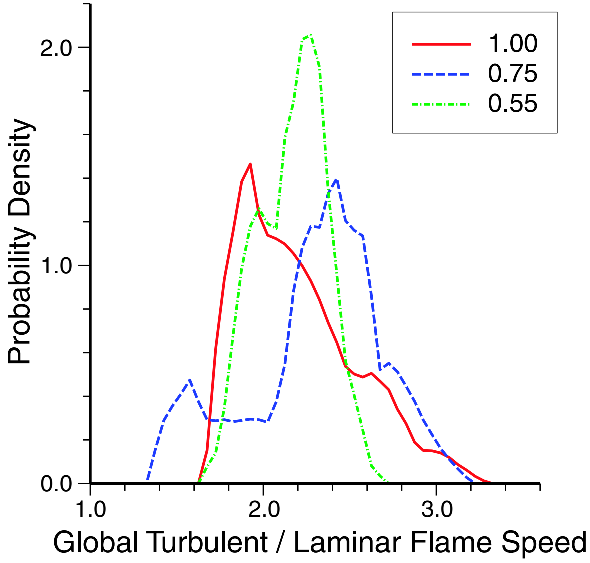
After stabilization, statistics over $\sim 5\ell_t/u'$

Typical 2D controlled flame surface

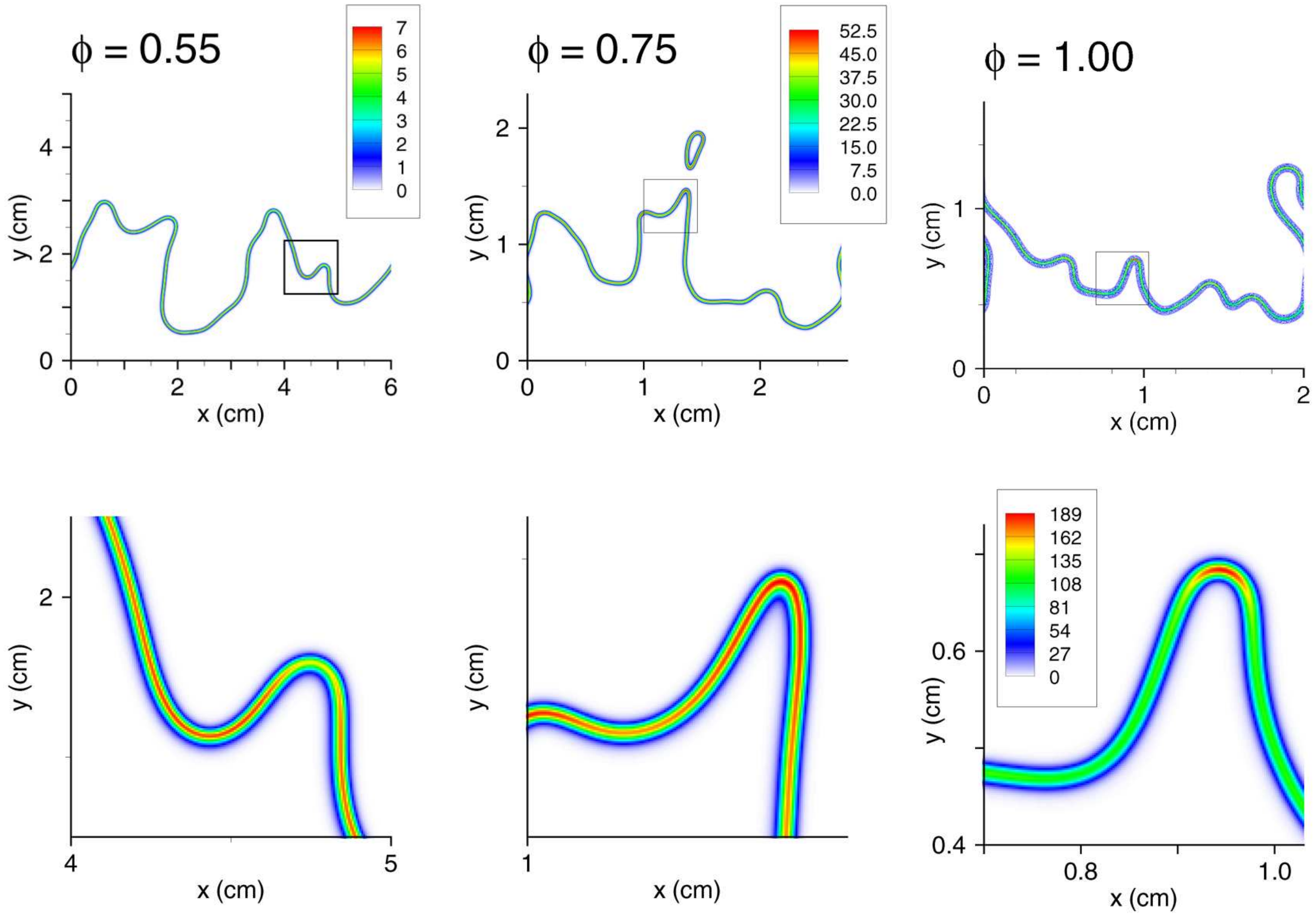


Contour of $T(Q_{max})$

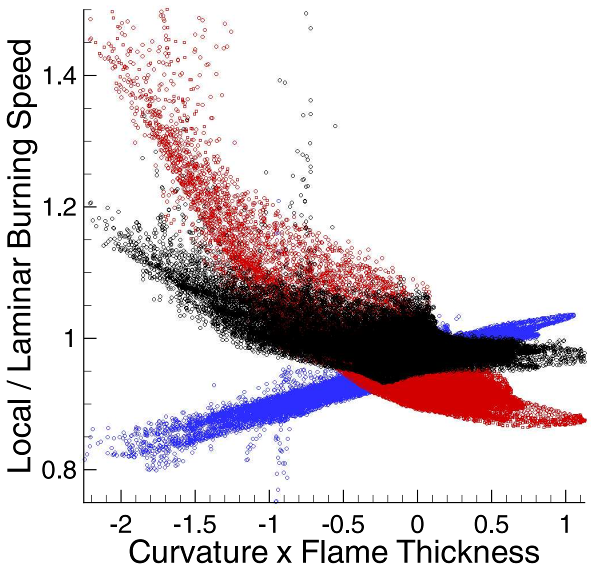


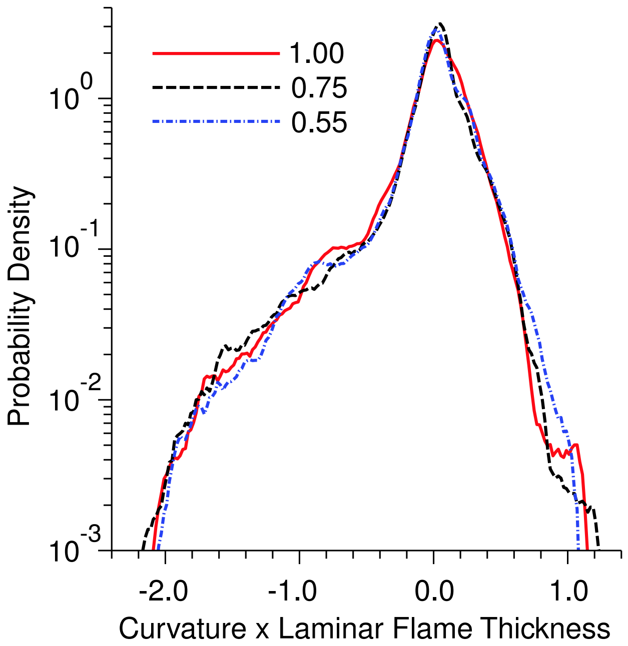


Consumption Rate Variability



Local Flame Analysis





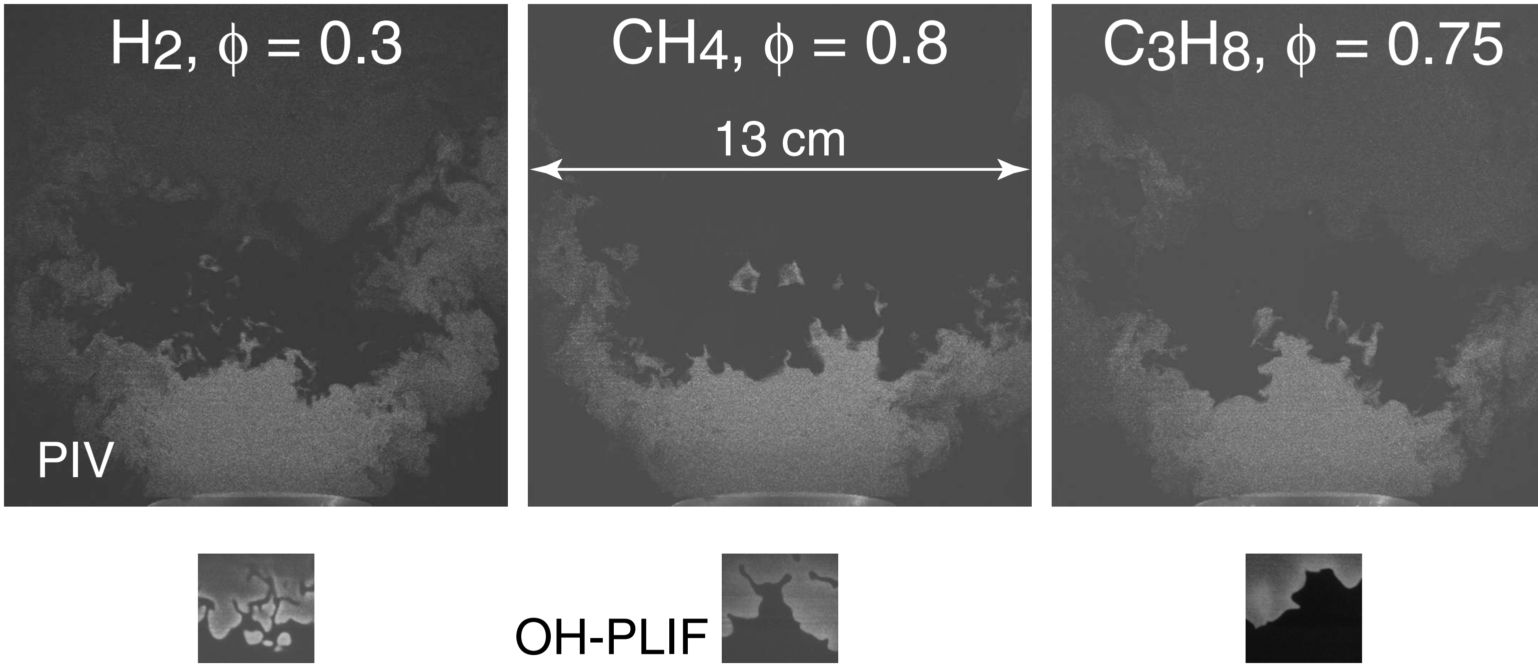
Use chemistry/transport detail and turbulence statistics to explain:

1. Correlation shift with mixture fraction, ϕ
2. Identical (scaled) curvature range/statistics

Collaboration with van Oijen/Bastiaans/de Goey
Technische Universiteit Eindhoven, The Netherlands
Advanced flamelet models based on integrals of "stretch" through flame

Thermo-diffusive Effects

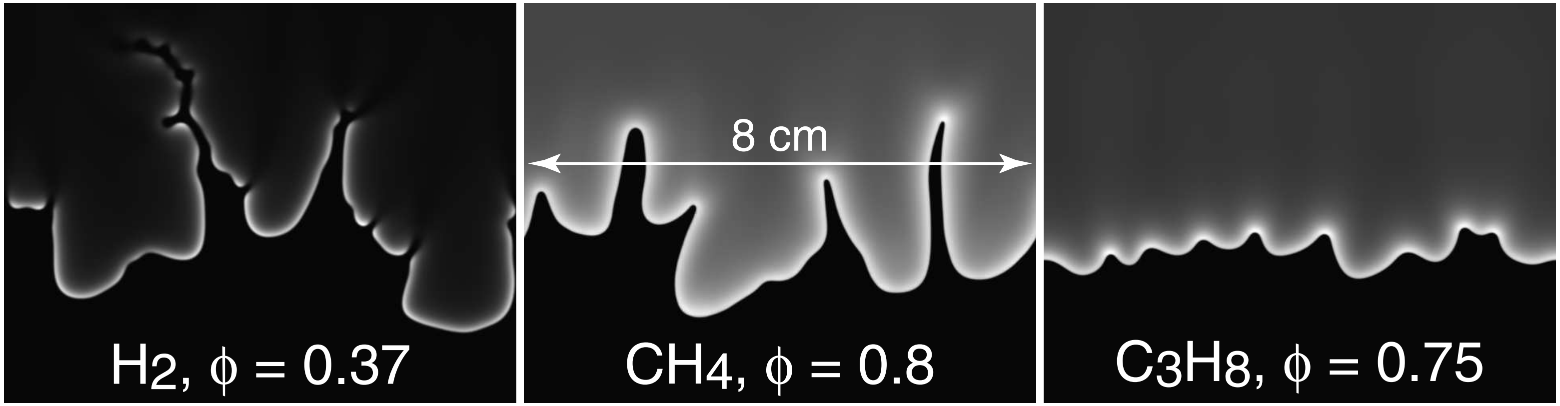
Flame wrinkle structures from low-swirl experiment



- Identical fueling rate/turbulence, range of burning modes due to thermo-diffusive instability of light fuel.
- (Apparent) local extinction, how to analyze experimental data?
- Can we use simulation to help understand these flames?

Control Application

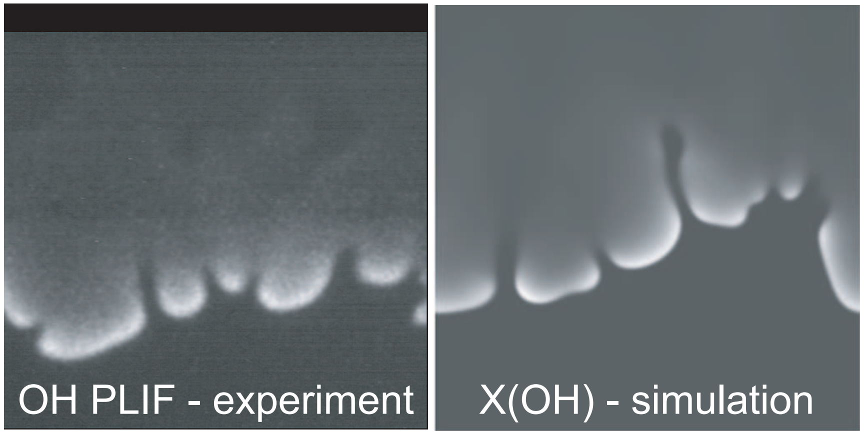
Use computational flame-control algorithm to study dynamics of flame surfaces in the central region of low-swirl burner experiments without the complexity of the LSB nozzle flow details



- 2D controlled flames: three fuels (molecular weight) (turbulence/fuels correspond roughly to experimental data)
- Simple systems reproduce observed wrinkling behaviour
- Use 3D simulation to characterize local extinction, wrinkle-suppression, etc.

Thermo-diffusive Effects

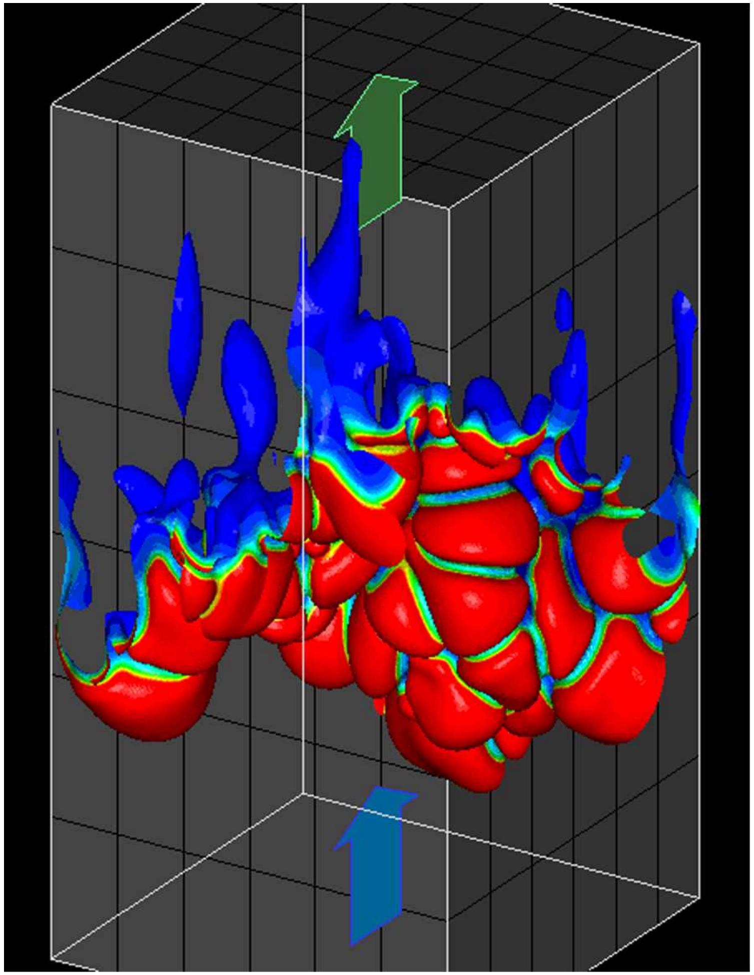
Early 3D results



3D controlled hydrogen flame

- Detailed/resolved chemistry, differential diffusion
- Structure of turbulence/wrinkling, OH signal variability

$T = 1200$ surface
(color: consumption rate)

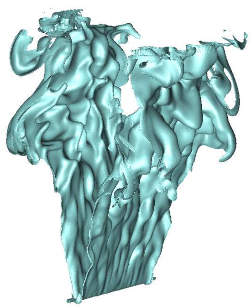


Extinction where highly curved
Click image for movie

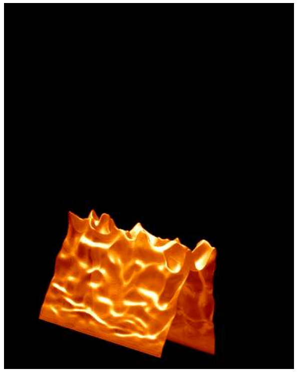
Ongoing Research

- Controlled TD unstable flame studies
  - Higher-order transport effects
- Collaboration with experimentalists:
  - Interpreting measured data
  - Experiments w/flame “isolation”

Click image for movie



Wire-Stabilized Flame
(Cheng, LBNL)



Slot Burner
(Driscoll, U. Mich.)

Flamelet model validation:

(w/van Oijen, et. al)

- 3D resolved flames
- Integrated stretch,
  $Ka \sim \int_{Flame} \kappa ds$
- To include Le_i effects