Verified Computations of Laminar Premixed Flames

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45^{th} AIAA Aerospace Science Meeting and Exhibit

Reno, Nevada

8 January 2007

UNIVERSITY OF NOTRE DAME

Objective

To obtain an accurate *a priori* estimate for the finest length scale in a continuum model of reactive flow with detailed kinetics and multi-component transport of:

- steady,
- one-dimensional,
- ideal gas mixture,
- premixed laminar flame.

Mathematical Model

Governing Equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial \tilde{t}} &= -\frac{\partial}{\partial \tilde{x}}(\rho \tilde{u}), \\
\frac{\partial}{\partial \tilde{t}}(\rho \tilde{u}) &= -\frac{\partial}{\partial \tilde{x}}\left(\rho \tilde{u}^2 + p - \tau\right), \\
\frac{\partial}{\partial \tilde{t}}\left(\rho\left(e + \frac{\tilde{u}^2}{2}\right)\right) &= -\frac{\partial}{\partial \tilde{x}}\left(\rho \tilde{u}\left(e + \frac{\tilde{u}^2}{2} + \frac{p}{\rho} - \frac{\tau}{\rho}\right) + J^q\right), \\
\frac{\partial}{\partial \tilde{t}}(\rho Y_i) &= -\frac{\partial}{\partial \tilde{x}}(\rho \tilde{u} Y_i + J_i^m) + \dot{\omega}_i M_i, \quad i = 1, \ldots, N-1.
\end{aligned}
$$

Constitutive Relations

$$J_i^m = \rho \sum_{\substack{k=1 \\ k \neq i}}^{N} \frac{M_i D_{ik} Y_k}{M} \left(\frac{1}{\chi_k} \frac{\partial \chi_k}{\partial \tilde{x}} + \left(1 - \frac{M_k}{M}\right) \frac{1}{p} \frac{\partial p}{\partial \tilde{x}} \right) - D_i^T \frac{1}{T} \frac{\partial T}{\partial \tilde{x}},$$

$$J^q = q + \sum_{i=1}^{N} J_i^m h_i - \Re T \sum_{i=1}^{N} \frac{D_i^T}{M_i} \left(\frac{1}{\chi_i} \frac{\partial \chi_i}{\partial \tilde{x}} + \left(1 - \frac{M_i}{M}\right) \frac{1}{p} \frac{\partial p}{\partial \tilde{x}} \right),$$

$$q = -k \frac{\partial T}{\partial \tilde{x}},$$

$$p = \Re T \sum_{i=1}^{N} \frac{\rho Y_i}{M_i},$$

and others . . .

Dynamical System Formulation

- PDEs $\longrightarrow$ ODEs

$$\begin{aligned}
\frac{d}{dx}(\rho u) &= 0, \\
\frac{d}{dx}(\rho u h + J^q) &= 0, \\
\frac{d}{dx}(\rho u Y_l^e + J_l^e) &= 0, \qquad l = 1, \ldots, L-1, \\
\frac{d}{dx}(\rho u Y_i + J_i^m) &= \dot{\omega}_i M_i, \qquad i = 1, \ldots, N-L.
\end{aligned}$$

- ODEs $\longrightarrow 2N+2$ DAEs

$$\mathbf{A}(\mathbf{z}) \cdot \frac{d\mathbf{z}}{dx} = \mathbf{f}(\mathbf{z}).$$

***A Posteriori* Length Scale Analysis**

- Standard eigenvalue analysis is not applicable; $\mathbf{A}$ is singular.

- The generalized eigenvalues can be calculated
  - from

$$\lambda \mathbf{A}^* \cdot \mathbf{v} \quad = \quad \mathbf{B}^* \cdot \mathbf{v},$$

  - and the length scales are given by

$$\ell_i = \frac{1}{|Re\,(\lambda_i)|}, \quad i = 1, \ldots, 2N - L.$$

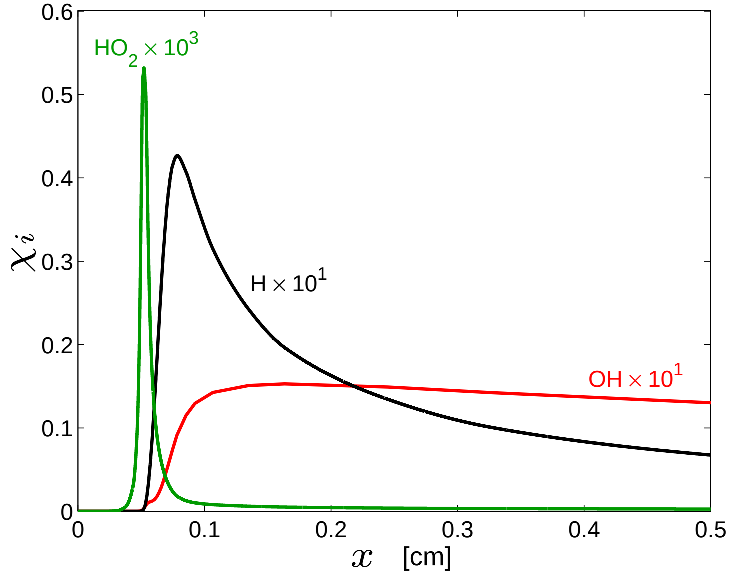
Results

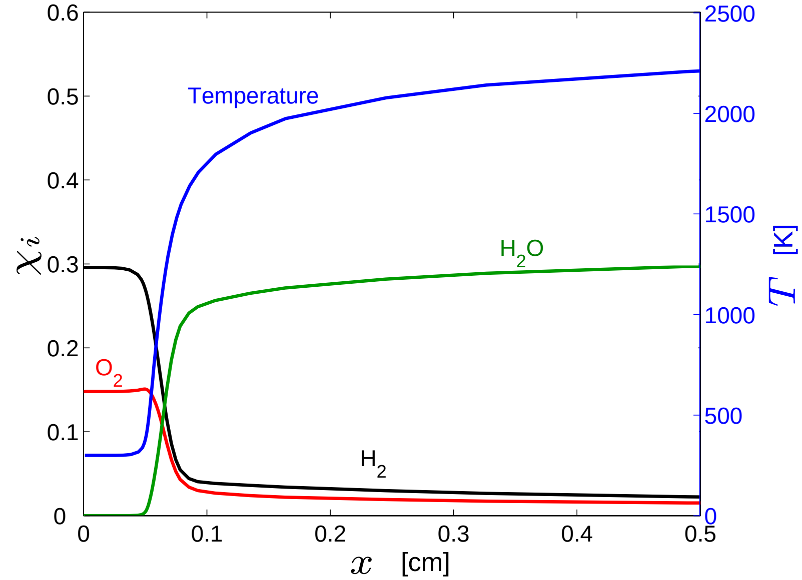
Steady Laminar Premixed Hydrogen-Air Flame

- $N = 9$ species, $L = 3$ atomic elements, and $J = 19$ reversible reactions,
- Stoichiometric Hydrogen-Air: $2H_2 + (O_2 + 3.76N_2)$,
- $T_{unburned} = 800\ K$,
- $p_o = 1\ atm$,
- CHEMKIN and IMSL are employed.

Mathematical Verification

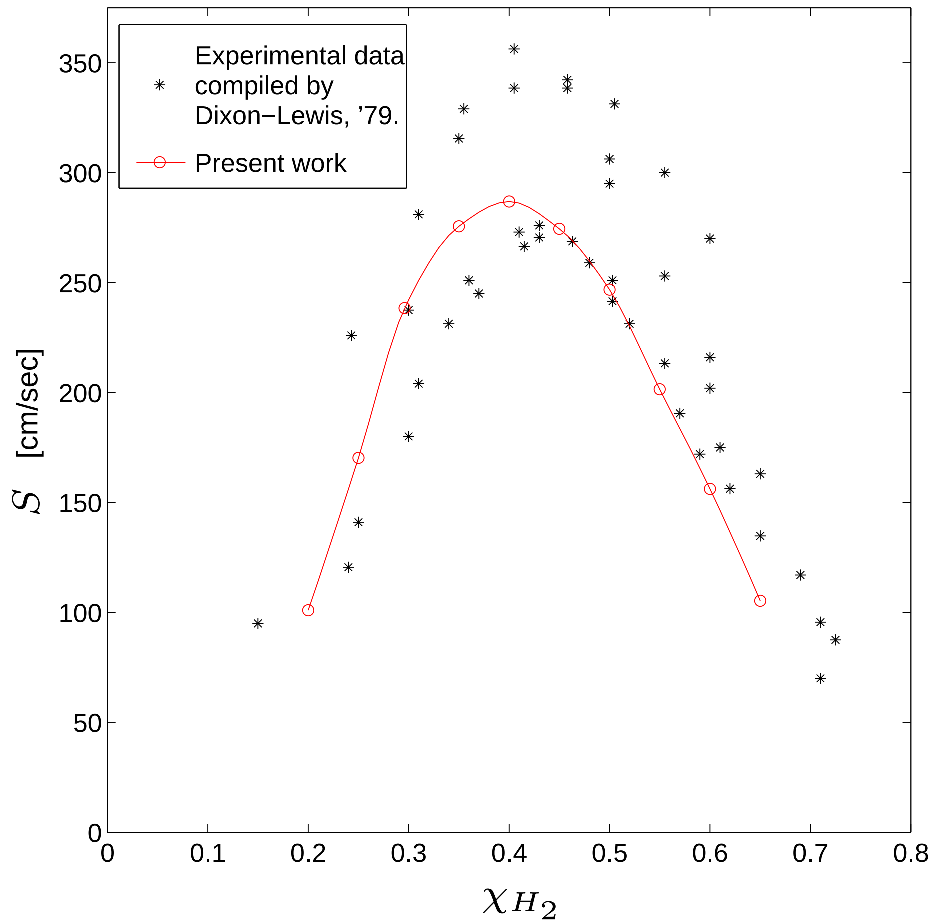
- Good agreement with *Smooke et al., ’83*.



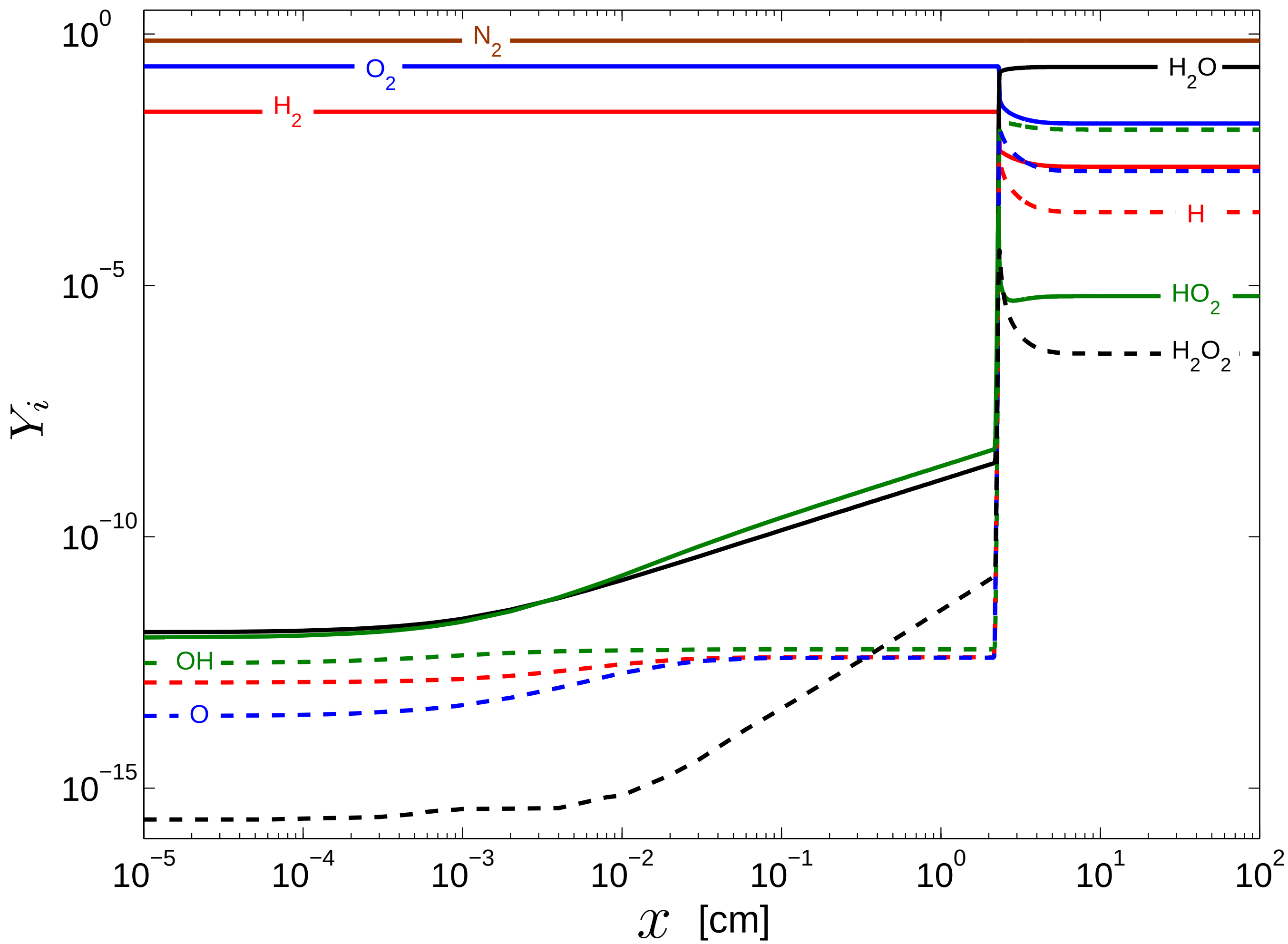


Experimental Validation

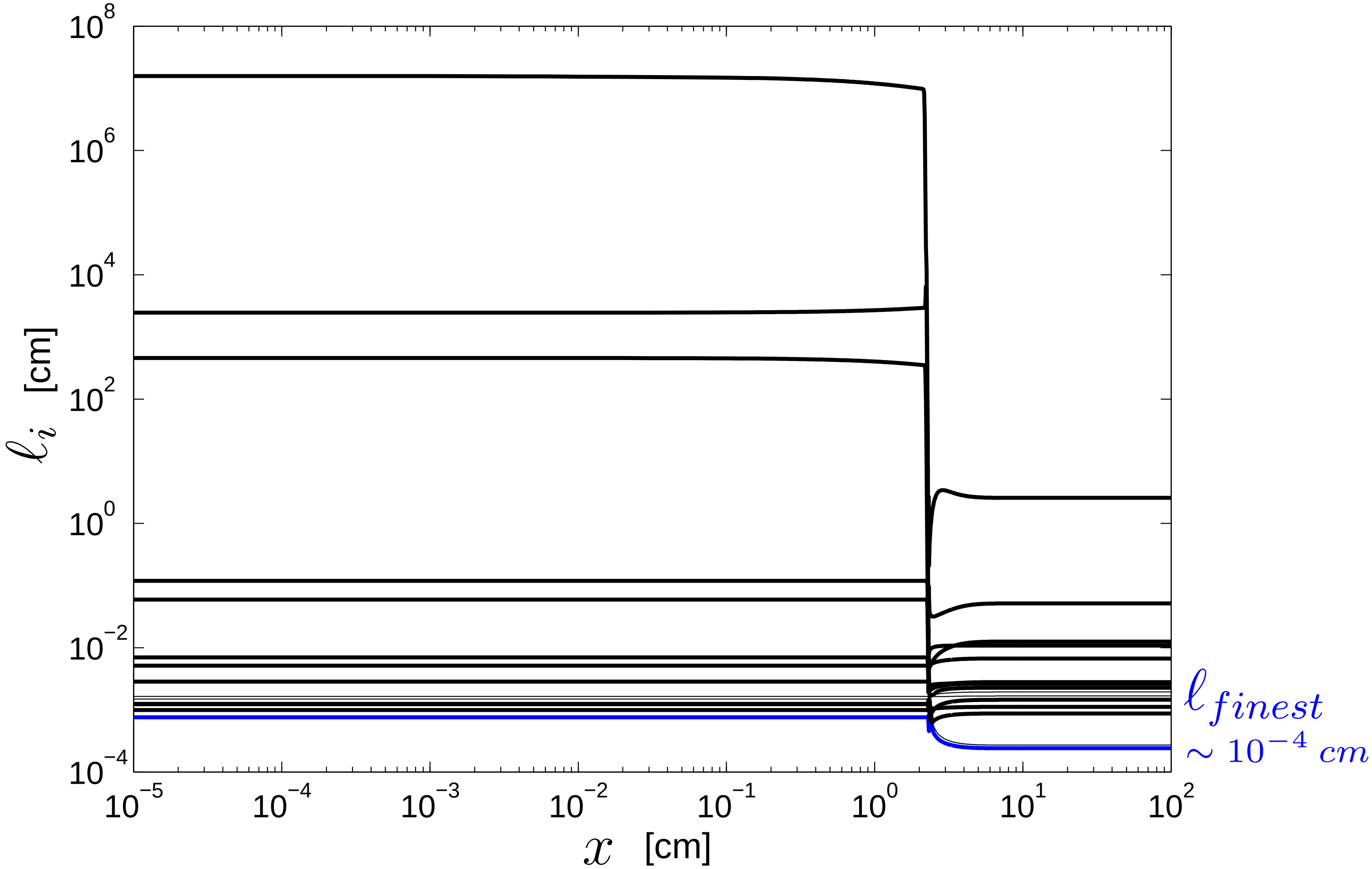
- Good agreement with Dixon-Lewis, '79.



Fully Resolved Structure



Predicted Length Scales



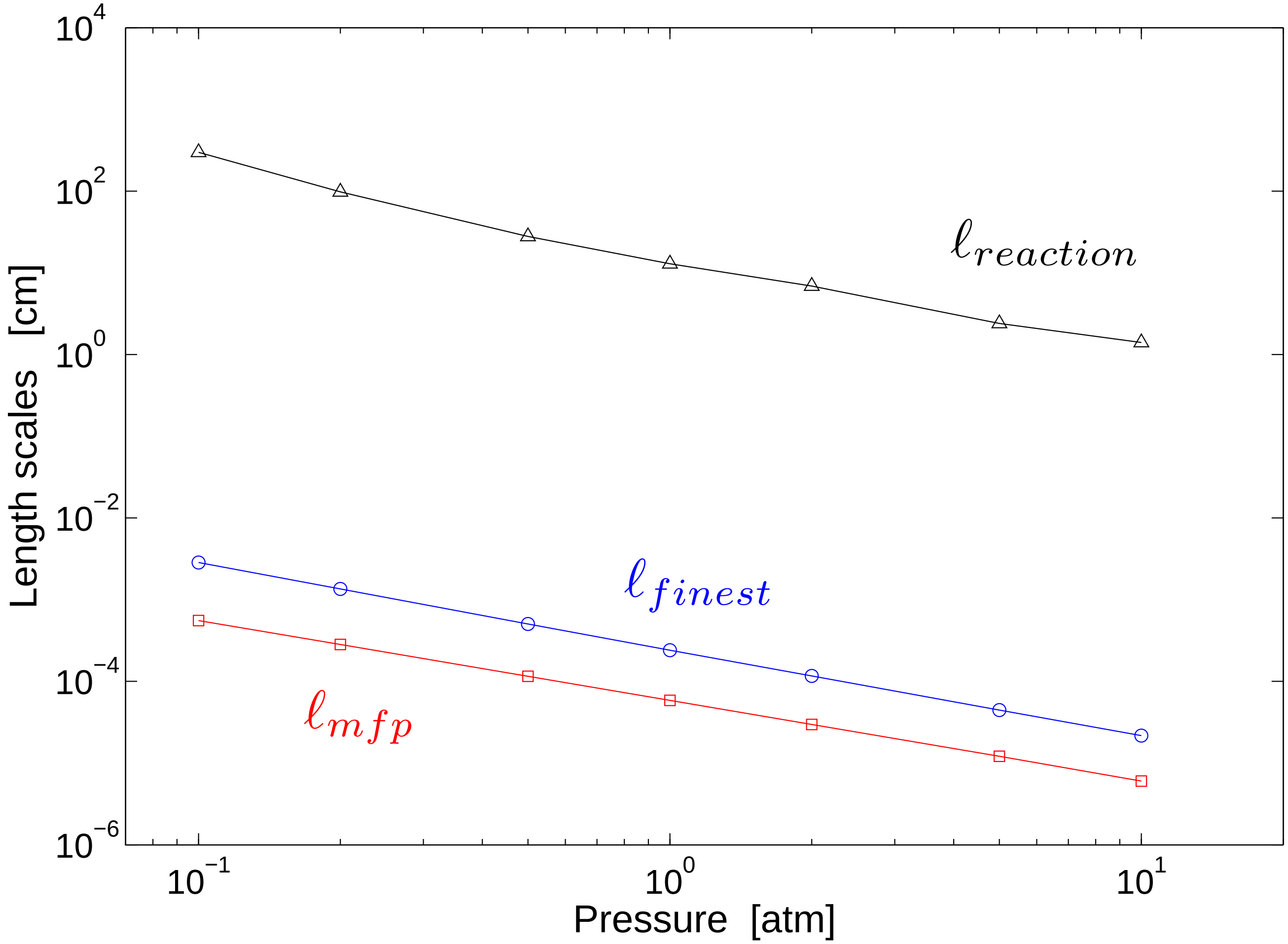
Mean-Free-Path Estimate

- The mixture mean-free-path scale is the cutoff *minimum* length scale associated with continuum theories.

- A simple estimate for this scale is given by *Vincenti and Kruger, '65*:

$$\ell_{mfp} = \frac{M}{\sqrt{2}\mathcal{N}\pi d^2 \rho}.$$

- ℓ_{finest} is well correlated with ℓ_{mfp}.

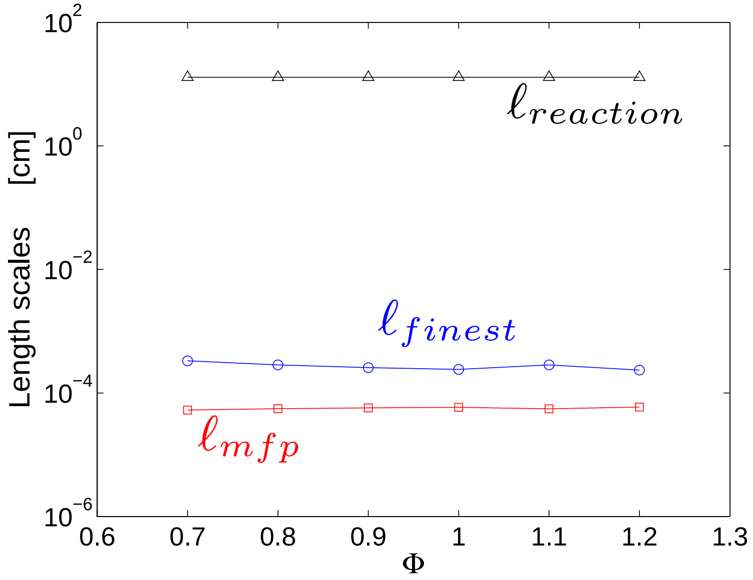


Extensions

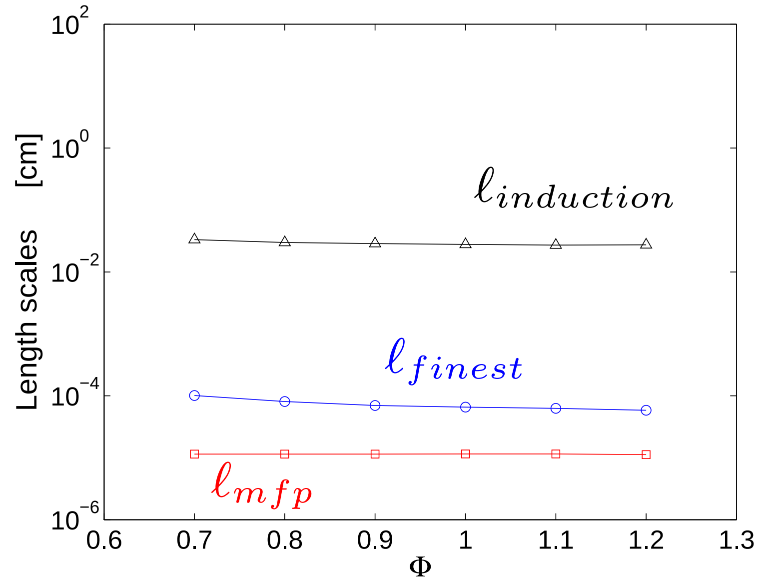
- Two additional sets of calculations:
  - Variable fuel/air ratio,
  - Hydrocarbon mixtures (methane, ethane, ethylene, acetylene).

- Two combustion regimes:
  - Freely propagating laminar flame,
  - Chapman-Jouguet detonation (*Powers and Paolucci, '05*).

Equivalence ratio influence is negligible

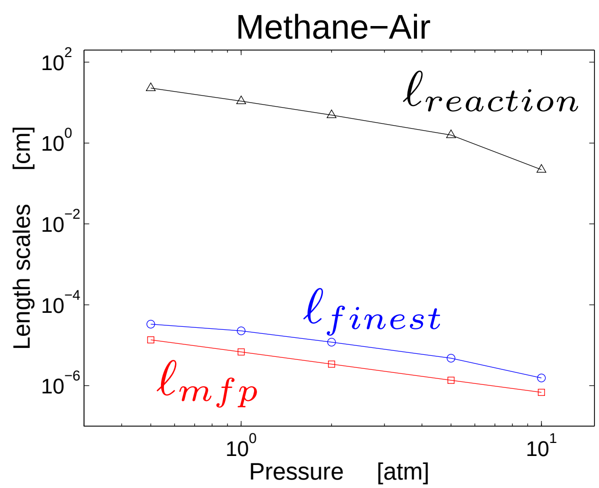


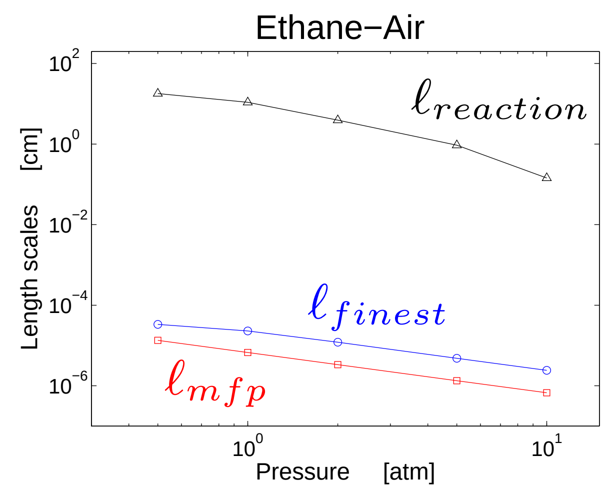
(a) Laminar premixed flame

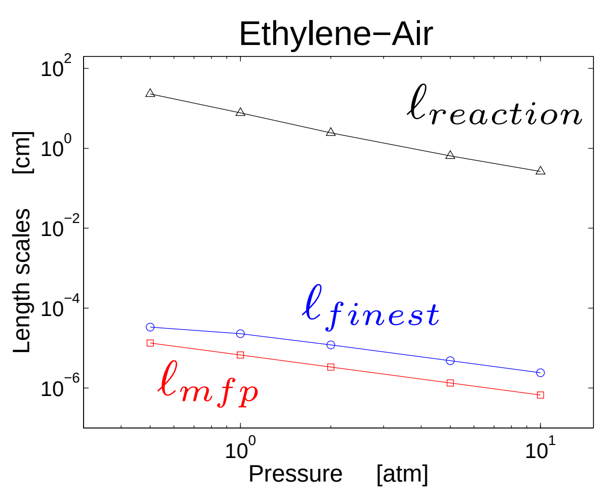


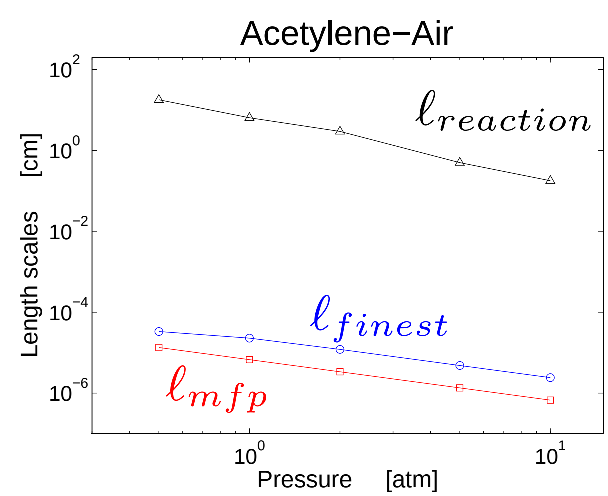
(b) Chapman-Jouguet detonation

Deflagration

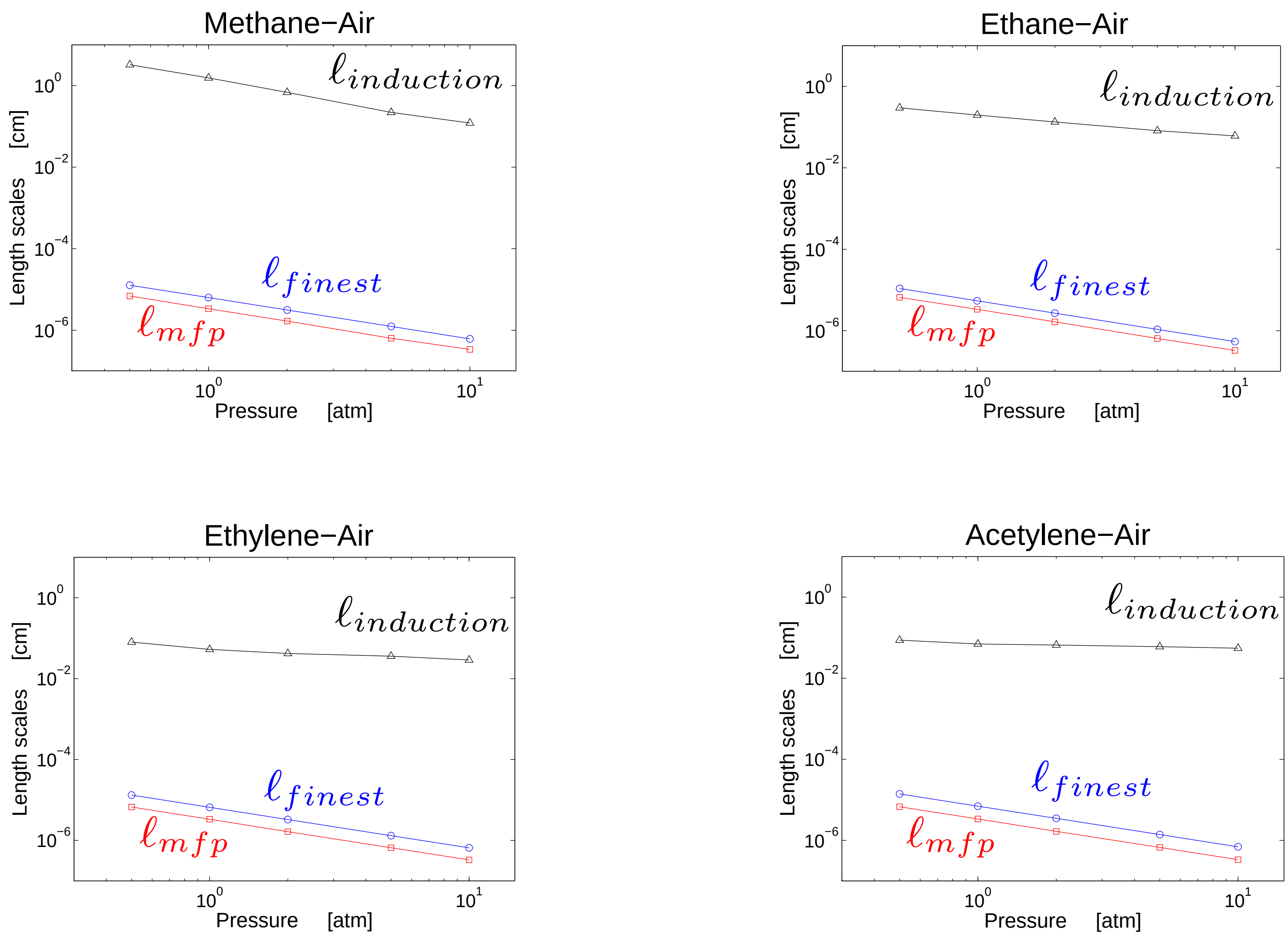








Detonation



Methane−Air
Ethane−Air
Ethylene−Air
Acetylene−Air
Length scales [cm]
Pressure [atm]
10^0
10^{-2}
10^{-4}
10^{-6}
10^1
$\ell_{induction}$
ℓ_{finest}
ℓ_{mfp}

Comparison with Published Results

Ref.	Mixture molar ratio	$\Delta x, (cm)$	$\ell_{finest}, (cm)$	$\ell_{mfp}, (cm)$
1	$1.26H_2 + O_2 + 3.76N_2$	2.50×10^{-2}	8.05×10^{-4}	4.33×10^{-5}
2	$CH_4 + 2O_2 + 10N_2$	unknown	6.12×10^{-4}	4.33×10^{-5}
3	$0.59H_2 + O_2 + 3.76N_2$	3.54×10^{-2}	4.35×10^{-5}	7.84×10^{-6}
4	$CH_4 + 2O_2 + 10N_2$	1.56×10^{-3}	2.89×10^{-5}	6.68×10^{-6}

1. Katta V. R. and Roquemore W. M., 1995, *Combustion and Flame*, **102** (1-2), pp. 21-40.
2. Najm H. N. and Wyckoff P. S., 1997, *Combustion and Flame*, **110** (1-2), pp. 92-112.
3. Patnaik G. and Kailasanath K., 1994, *Combustion and Flame*, **99** (2), pp. 247-253.
4. Knio O. M. and Najm H. N., 2000, *Proc. Combustion Institute*, **28**, pp. 1851-1857.

Discussion

A lower bound for the grid resolution is desirable

- Grid convergence, (*Roache, '98*).
  - Convergence rate must be consistent with truncation error order.
  - Grids coarser than the finest length scale could unphysically influence reaction dynamics.
- Direct numerical simulation (DNS).
  - Our results are in rough agreement with independent estimates found in DNS of reacting flows, $\Delta x = 4.30 \times 10^{-4}\, cm$, (*Chen et al., '06*).

The modified equation for a model problem

$$\begin{aligned} \frac{\partial\psi}{\partial t} + a\frac{\partial\psi}{\partial x} &= \nu\frac{\partial^2\psi}{\partial x^2}, \\ \frac{\psi_i^{n+1}-\psi_i^n}{\Delta t} + a\frac{\psi_i^n-\psi_{i-1}^n}{\Delta x} &= \nu\frac{\psi_{i+1}^n-2\psi_i^n+\psi_{i-1}^n}{\Delta x^2}, \end{aligned}$$

$$\begin{aligned} \frac{\partial\psi}{\partial t} + a\frac{\partial\psi}{\partial x} = & \left(\nu + \underbrace{\frac{a\Delta x}{2}\left(1-\frac{a\Delta t}{\Delta x}\right)}_{\text{leading order numerical diffusion}}\right)\frac{\partial^2\psi}{\partial x^2} \\ & + \underbrace{\frac{a\Delta x^2}{6}\left(-1+\left(\frac{a\Delta t}{\Delta x}\right)^2+6\frac{\nu\Delta t}{\Delta x^2}\right)}_{\text{leading order numerical dispersion}}\frac{\partial^3\psi}{\partial x^3} + \ldots \end{aligned}$$

- Discretization-based terms alter the dynamics.
- Numerical diffusion could suppress physical instability.

- To solve for the steady structure

$$
\begin{aligned}
a\frac{d\psi}{dx} &= \nu\frac{d^2\psi}{dx^2}, \\
\text{Exact solution} \Rightarrow \psi &= C_1 + C_2 \exp\left(\frac{ax}{\nu}\right).
\end{aligned}
$$

  - Analogous to what has been done in our work

$$
\begin{aligned}
\lambda &= [0 \quad a/\nu], \\
\Rightarrow \ell_{finest} &= \nu/a.
\end{aligned}
$$

  - The required grid resolution is $\Delta x < \nu/a$.

- This grid size guarantees that the steady parts of the dissipation and dispersion errors in the model problem are small.

Implications for combustion

- Equilibrium quantities are insensitive to resolution of fine scales.
- Due to non-linearity, errors at micro-scale level may alter the macro-scale behavior.
- The sensitivity of results to fine scale structures is not known *a priori*.
- Lack of resolution may explain some failures, e.g. DDT.
- Linear stability analysis:
  - Requires the fully resolved steady state structure.
  - For one-step kinetics, *Sharpe, '03* shows failure to resolve steady structures leads to quantitative and qualitative errors in premixed laminar flame dynamics.

Conclusions

- To formally resolve the one-dimensional steady reactive flow, micron-level resolution is needed.
- Results will likely hold for multi-dimensional unsteady flows.
- The finest length scales are fully reflective of the underlying physics and not the particular mixture, chemical kinetics mechanism, or numerical method.
- The required grid resolution can be easily estimated *a priori* by a simple mean-free-path calculation.
- Present steady results cannot show where unsteady models will fail, but accurate capture of bifucation dynamics will likely require capture of all scales.