Verification and Validation of Premixed Laminar Flames

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Objectives

- To give detailed evidence that a mathematically verified estimate for the finest length scale in a continuum model of a premixed laminar flame with detailed kinetics is $\mathcal{O}(10^{-4}\ cm)$.
- To show such a continuum model can be macro-validated by comparing predictions of flames speeds to observations, while noting $10^{-4}\ cm$-scale structures are too fine for present-day combustion diagnositics.

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

$$
\begin{aligned}
J_i^m &= \rho \sum_{\substack{k=1\\k\neq i}}^{N} \frac{M_i D_{ik} Y_k}{M} \left(\frac{1}{\chi_k} \frac{\partial \chi_k}{\partial \tilde{x}} + \left(1 - \frac{M_k}{M}\right) \frac{1}{p} \frac{\partial p}{\partial \tilde{x}} \right) - D_i^T \frac{1}{T} \frac{\partial T}{\partial \tilde{x}}, \\
J^q &= q + \sum_{i=1}^{N} J_i^m h_i - \Re T \sum_{i=1}^{N} \frac{D_i^T}{M_i} \left(\frac{1}{\chi_i} \frac{\partial \chi_i}{\partial \tilde{x}} + \left(1 - \frac{M_i}{M}\right) \frac{1}{p} \frac{\partial p}{\partial \tilde{x}} \right), \\
\dot{\omega}_i &= \sum_{j=1}^{J} \nu_{ij} a_j T^{\beta_j} \exp\left(\frac{-\overline{E}_j}{\overline{R} T} \right) \left(\prod_{k=1}^{N} \overline{\rho}_k^{\nu'_{kj}} \right) \left(1 - \frac{1}{K_{c,j}} \prod_{k=1}^{N} \overline{\rho}_k^{\nu_{kj}} \right) \\
q &= -k \frac{\partial T}{\partial \tilde{x}}, \\
p &= \Re T \sum_{i=1}^{N} \frac{\rho Y_i}{M_i},
\end{aligned}
$$

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 $\longrightarrow$ DAEs

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

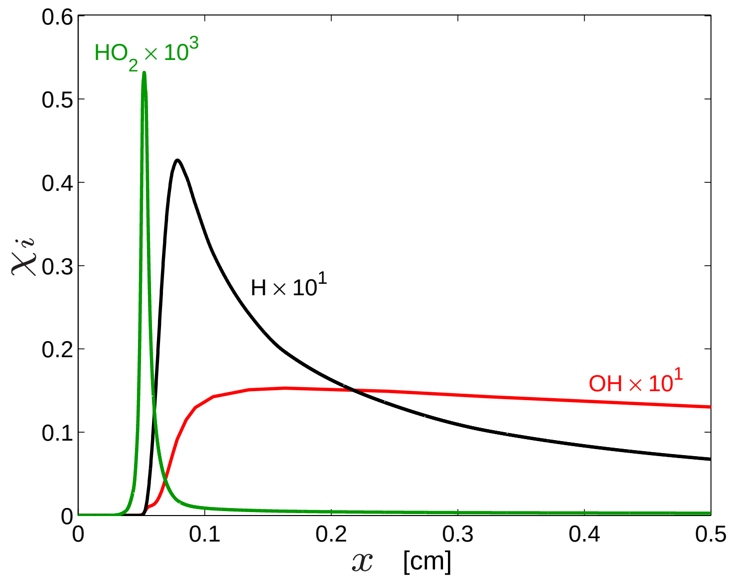
Results

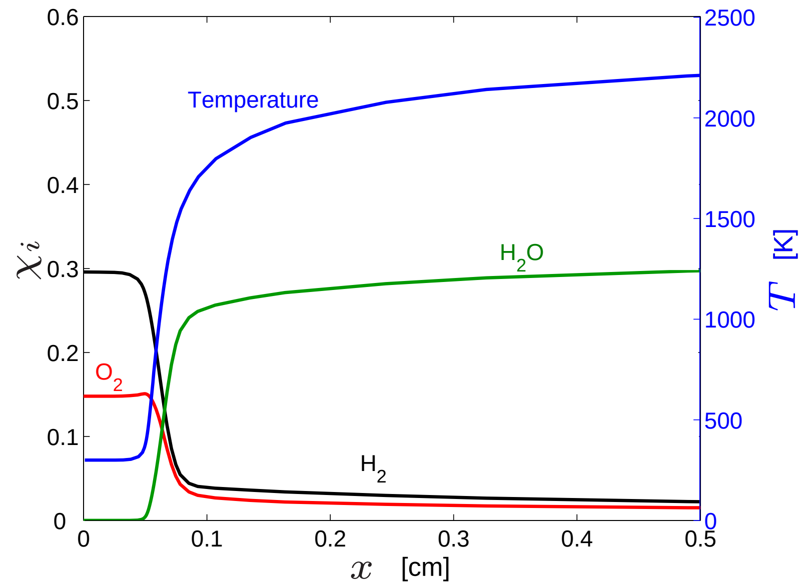
Steady Laminar Premixed Hydrogen-Air Flame

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

Macro-Mathematical Verification

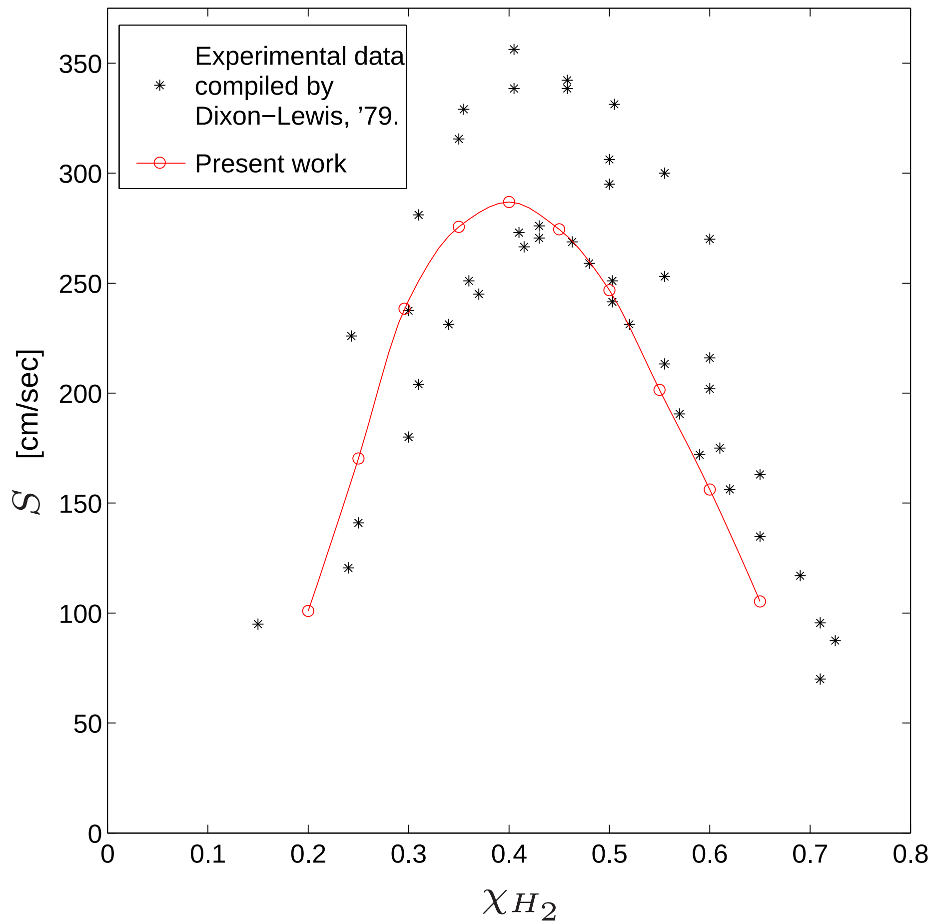
- Good “picture norm” agreement with Smooke *et al.*, ‘83.





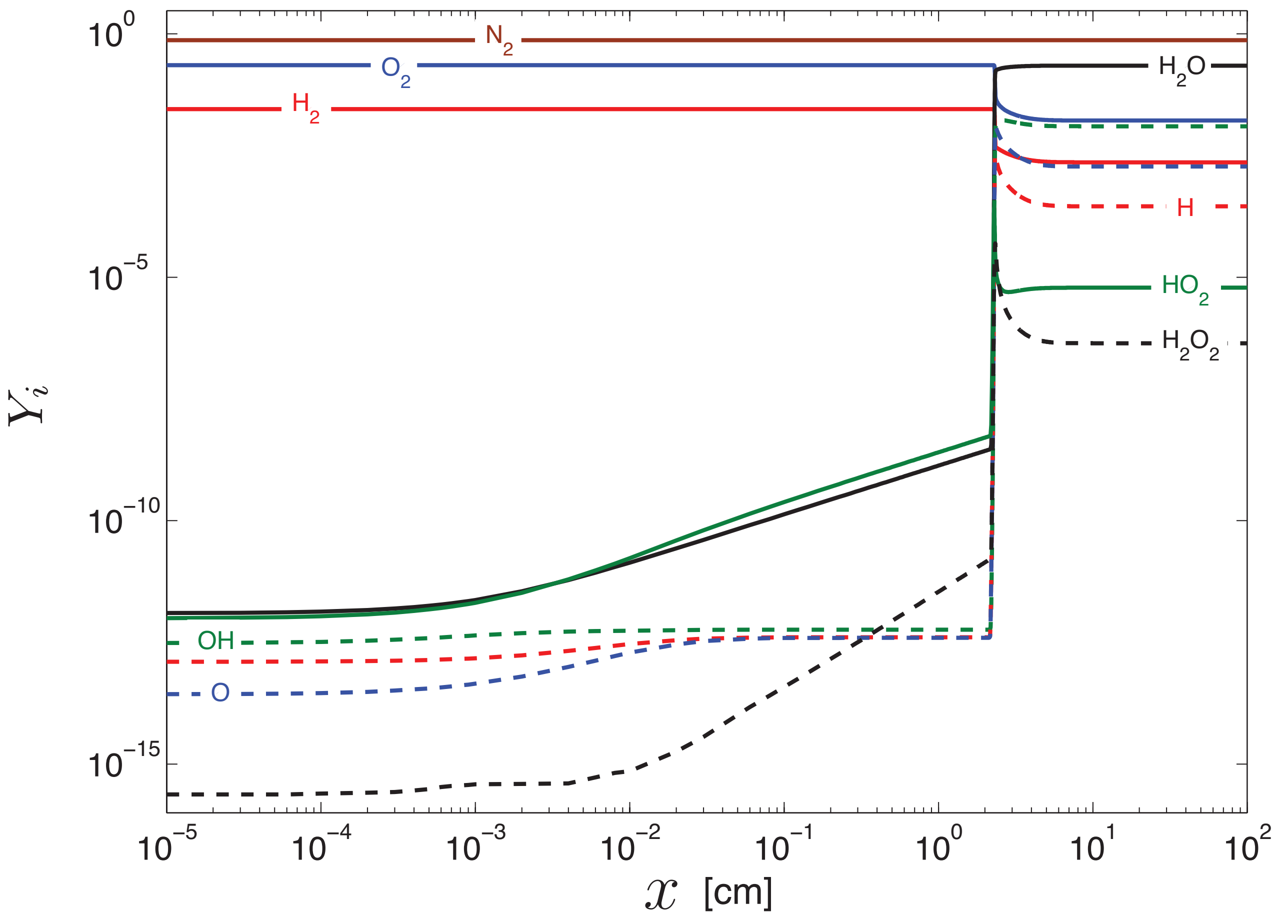
Macro-Experimental Validation

- Good agreement with flame speed data (Dixon-Lewis, ’79).



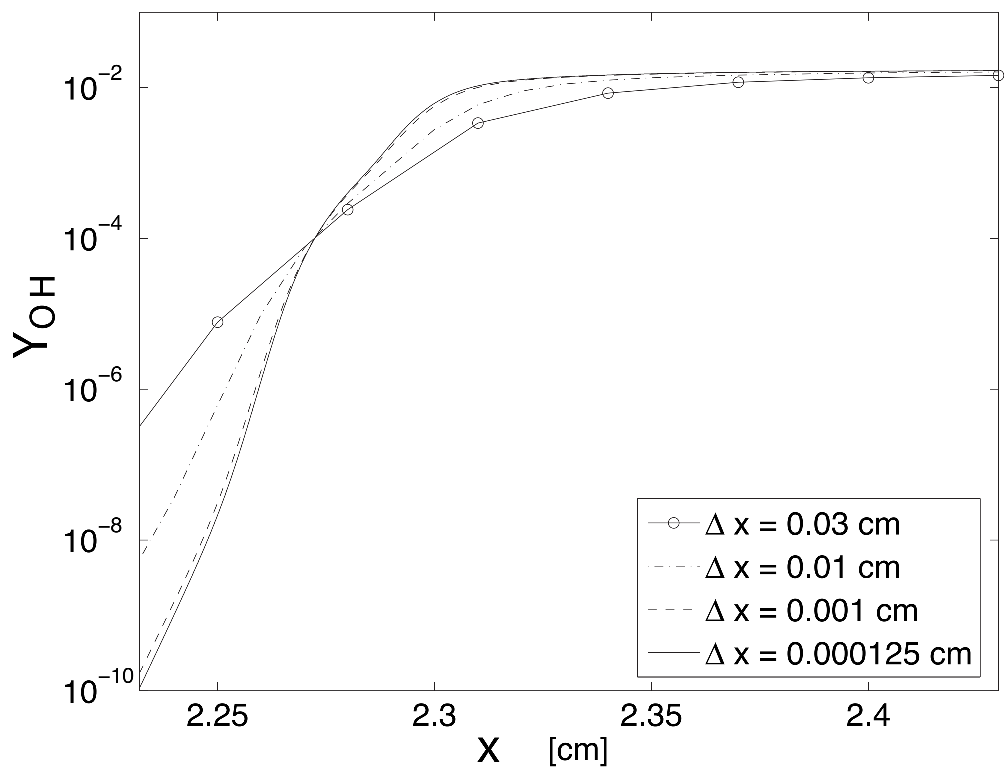
Micro-verification: log-log plot reveals structure at $10^{-4}\ cm$

- mass fractions versus distance

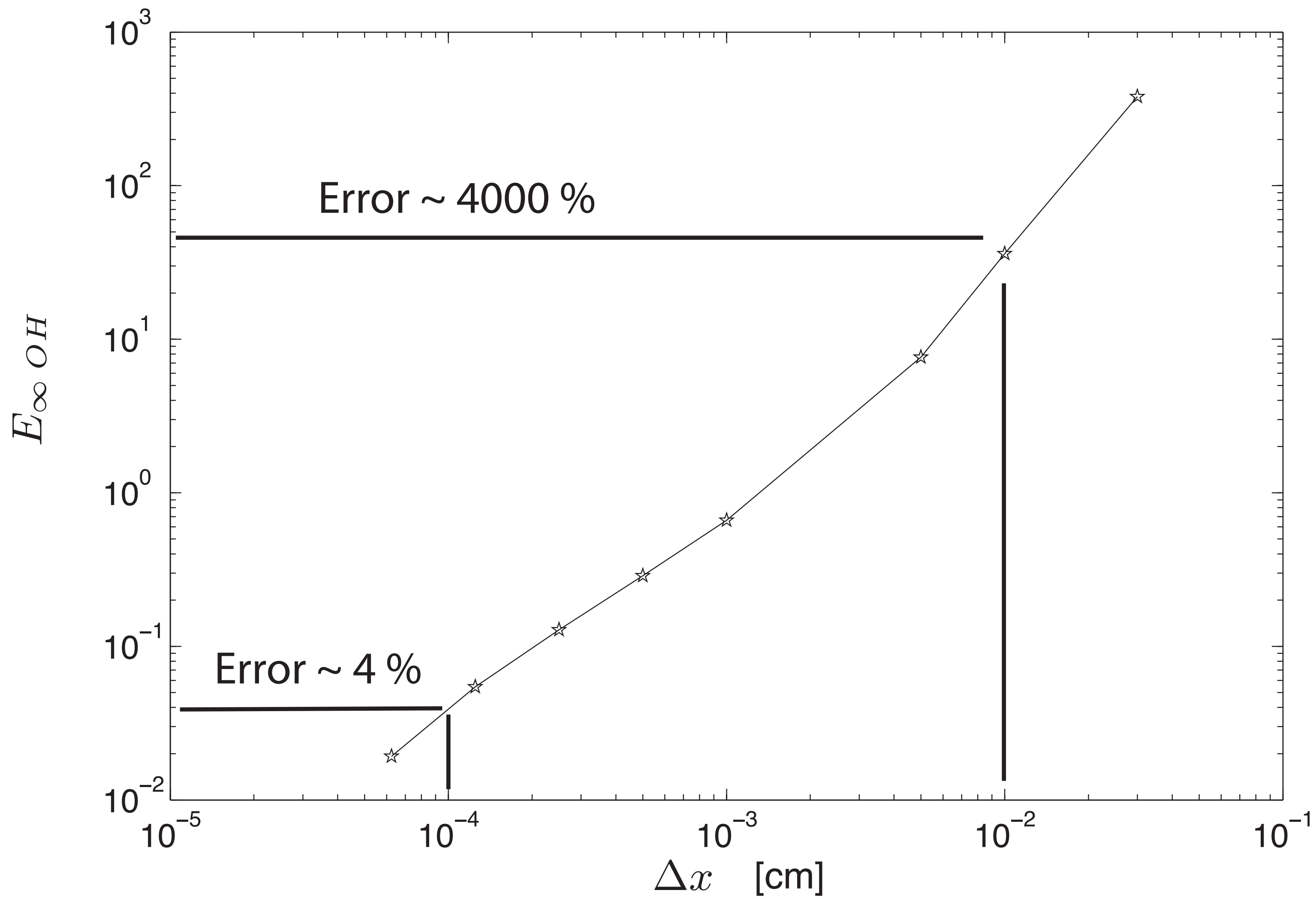


Variation of grid shows physical scales are at $O(10^{-4})\ cm$

- 4000% error in Y_{OH} when $\Delta x = 10^{-2}\ cm$!
- 4% error in Y_{OH} at $\Delta x \sim 10^{-4}\ cm$.

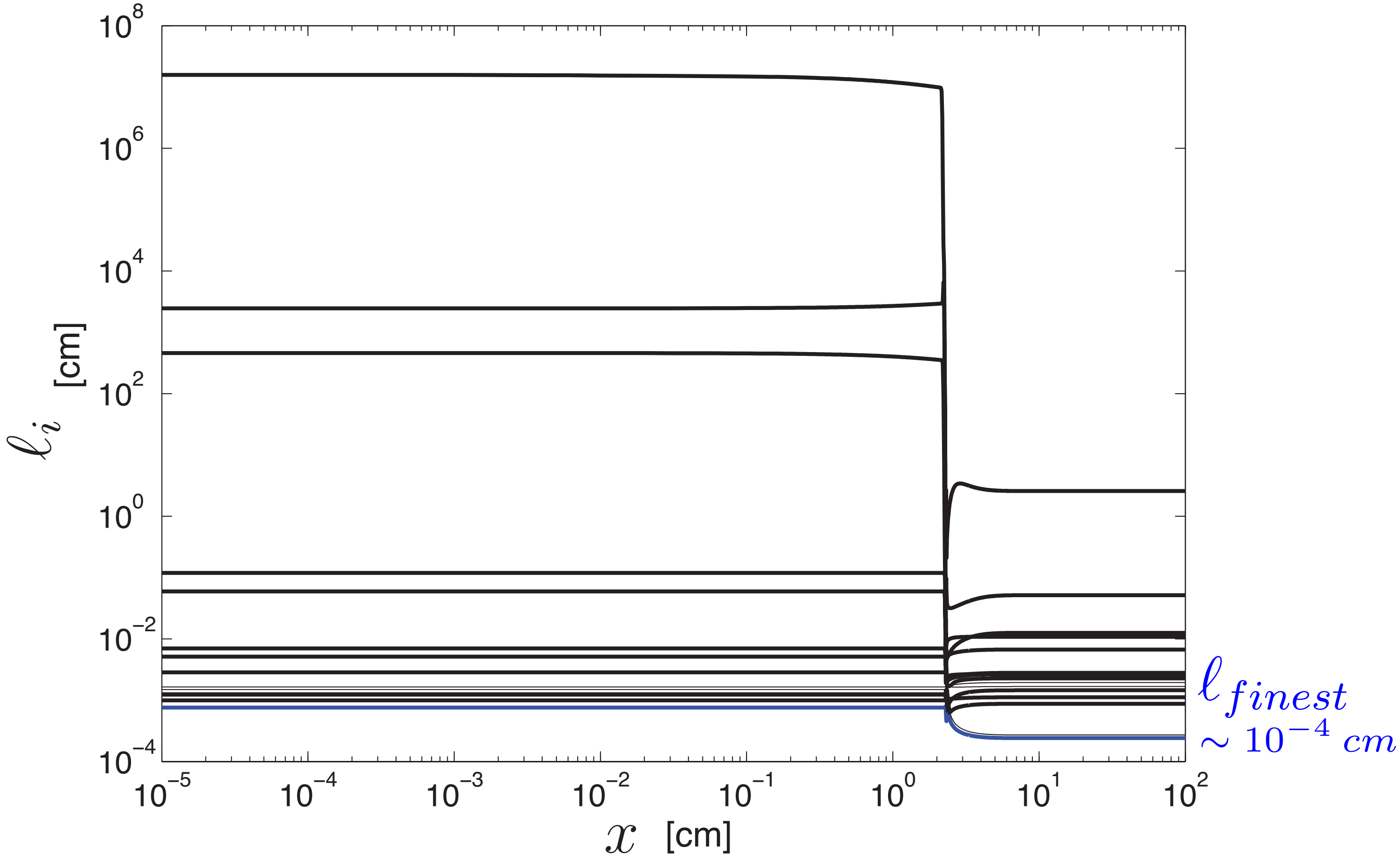


Grid convergence shows physical scales are at $O(10^{-4})\ cm$



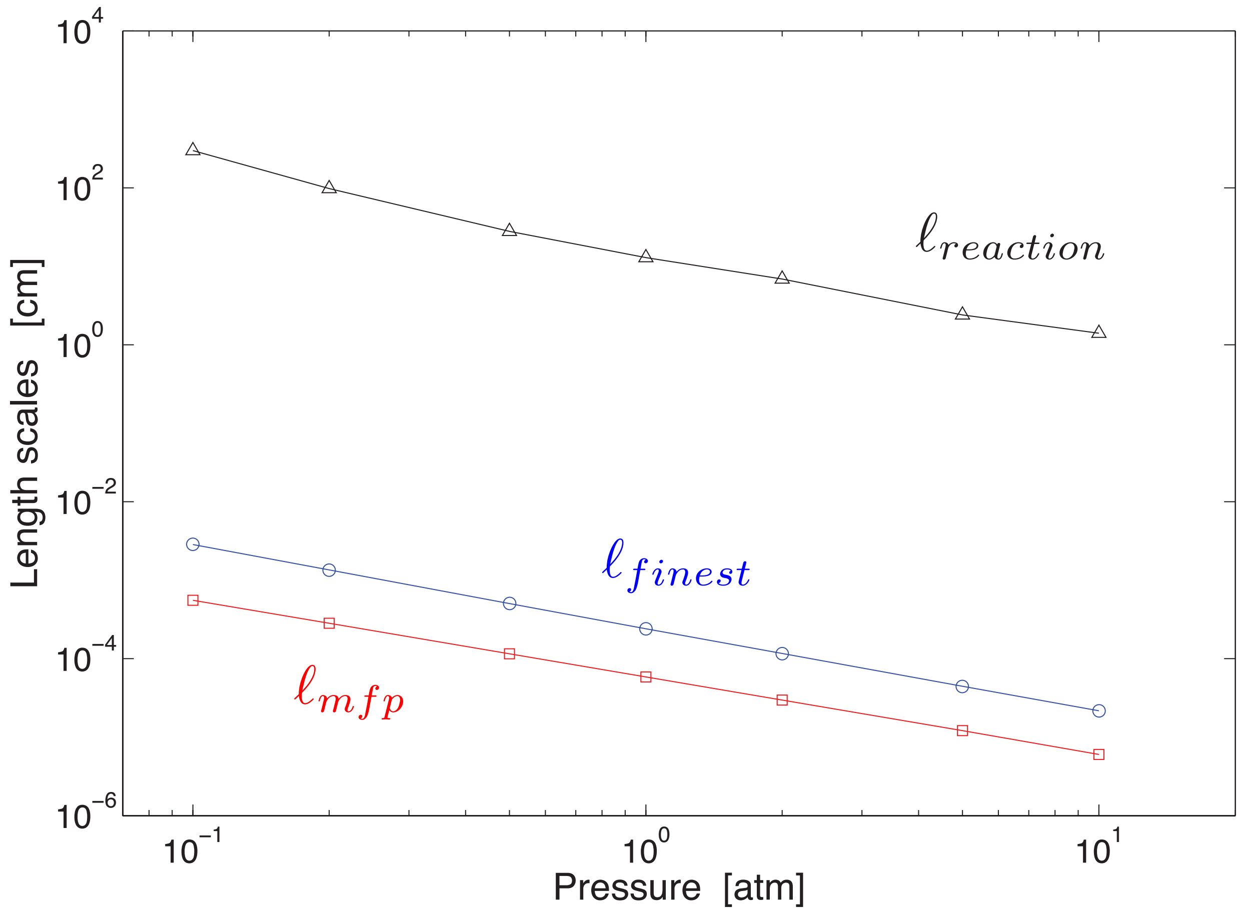
Spatial eigenvalue analysis shows scales are $O(10^{-4})\ cm$

- Found from generalized eigenvalues of $\mathbf{A}(\mathbf{z}) \cdot d\mathbf{z}/dx = \mathbf{f}(\mathbf{z})$.

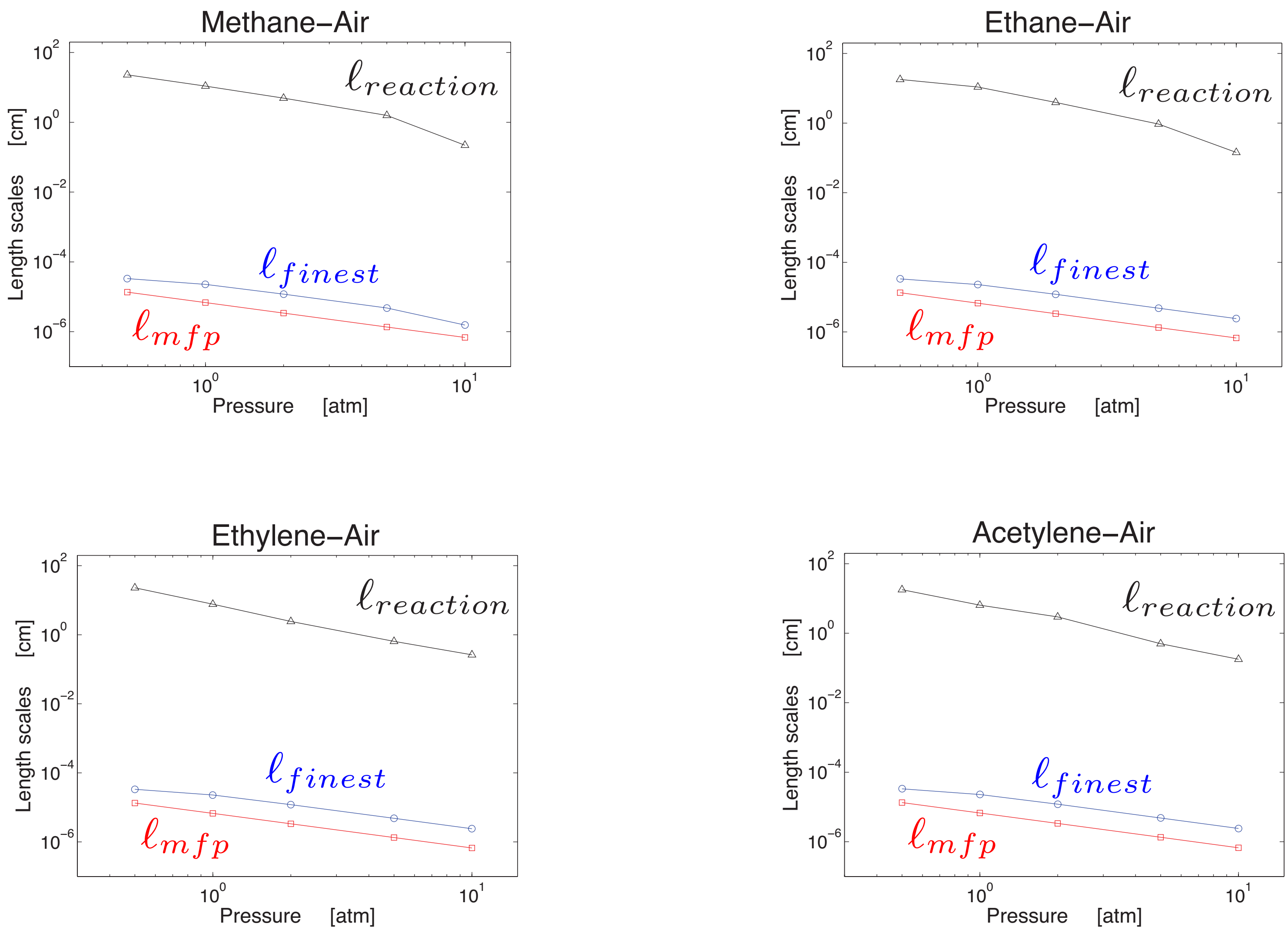


Mean free path estimates shows scales are $O(10^{-4})\ cm$

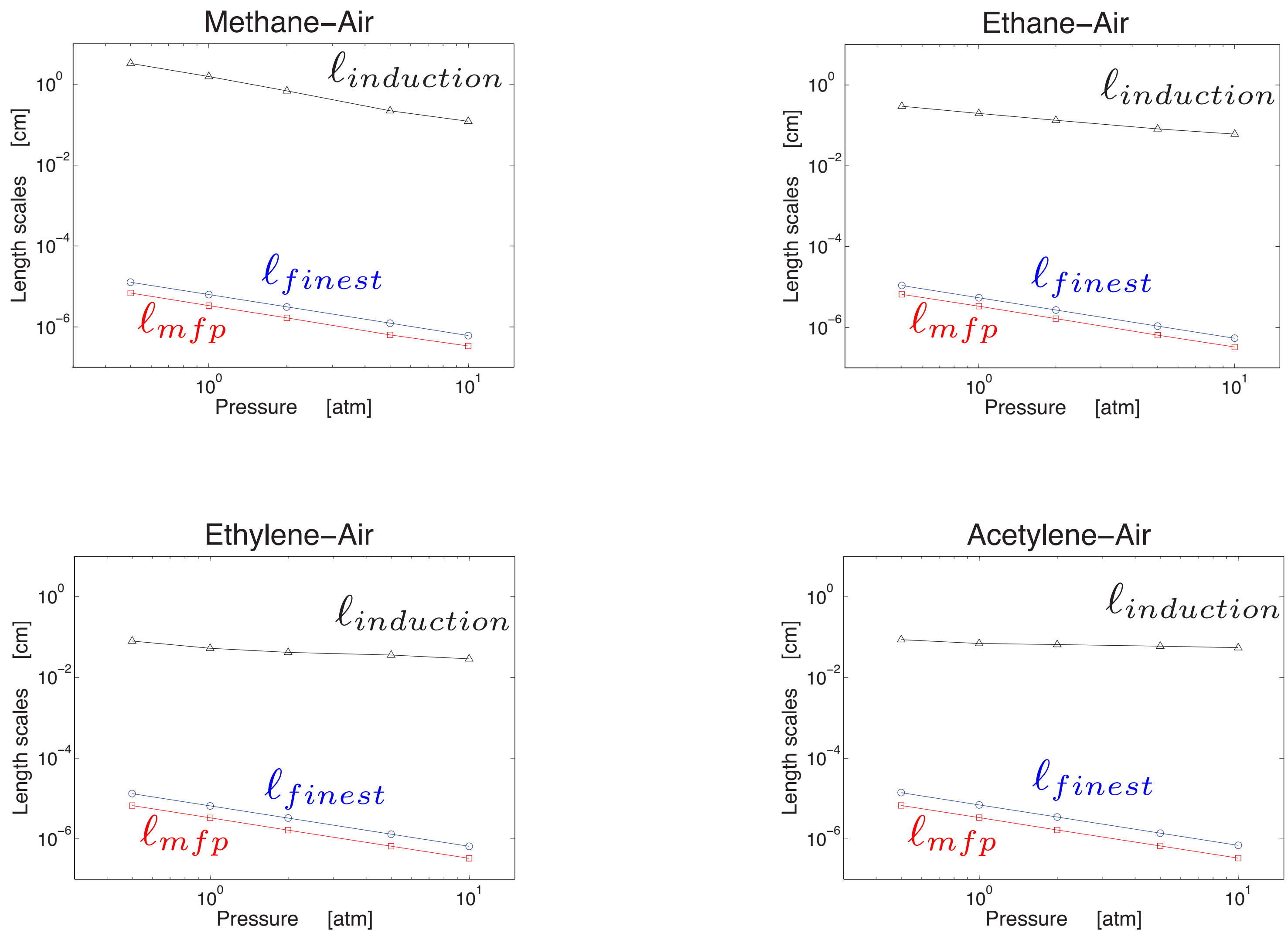
- $\ell_{mfp} = \frac{M}{\sqrt{2}\mathcal{N}\pi d^2\rho}$, the cutoff scale for continuum theory.



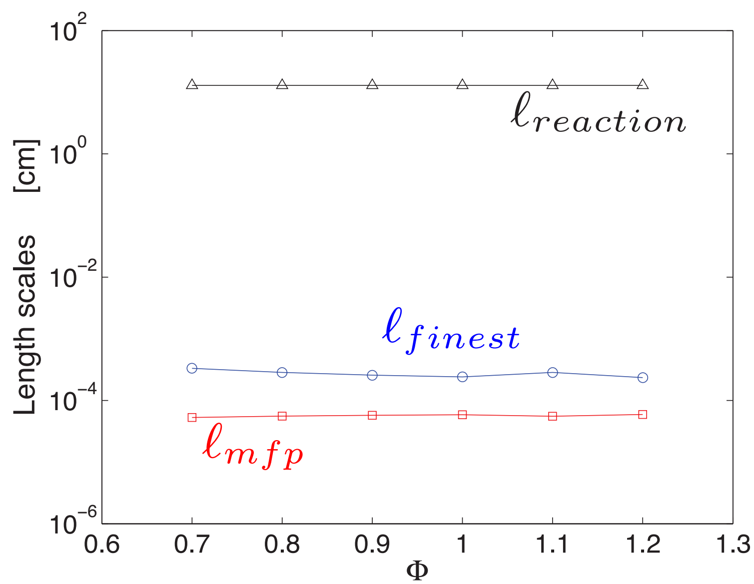
Hydrocarbon deflagration has scales at $10^{-4}\ cm$



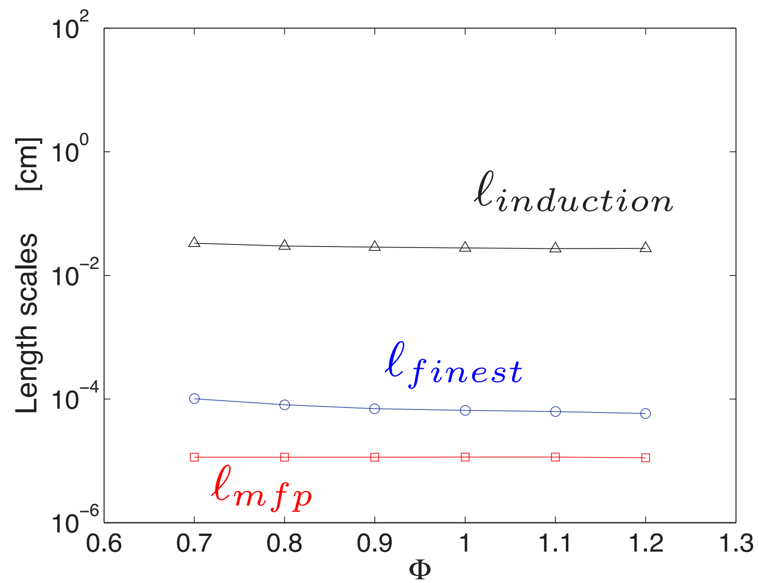
Hydrocarbon detonation has scales at $10^{-4}\ cm$



Variable equivalence ratio gives scales at $10^{-4}\ cm$



(a) Laminar premixed flame



(b) Chapman-Jouguet detonation

Independent unsteady calculations show scales are $O(10^{-4})\ cm$

For recent DNS of unsteady hydrogen-air flames...

"The domain is $4.1\ mm$ in each of the two spatial directions. A uniform grid spacing of $4.3\ microns$ was required to resolve the ignition fronts..."

J. H. Chen, *et al.*, "Direct numerical simulation of ignition front propagation in a constant volume with temperature inhomogeneities. I. Fundamental analysis and diagnostics," *Combustion and Flame*, 145:128-144, 2006.

Comparison with Other 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.

The modified equation for a model problem

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

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

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

- To solve for the steady structure

$$a\frac{d\psi}{dx} = \nu\frac{d^2\psi}{dx^2},$$

$$\text{Exact solution} \Rightarrow \psi = C_1 + C_2 \exp\left(\frac{ax}{\nu}\right).$$

  - Analogous to what has been done in our work

$$\lambda = [0 \quad a/\nu],$$

$$\Rightarrow \ell_{finest} = \nu/a.$$

  - 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

- Verification of one-dimensional steady flames require $10^{-4}\ cm$-level resolution.
- Result holds for multi-dimensional unsteady flows (Chen, 2006).
- 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.
- Validation of steady one-dimensional flame speeds is not difficult.
- Validation of complex flame dynamics will likely require $10^{-4}\ cm$ resolution.