On the Coupling Between Length and Time Scales in Reactive Flow

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Objectives

- To illustrate the full coupling of length and time scales in reactive flows.
- To give evidence that a mathematically verified estimate for the finest length scale in a continuum model of a 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 diagnostics.

Scale Coupling in Paradigm Linear System

- $$\underbrace{\frac{\partial\psi}{\partial t}}_{\text{evolution}} + \underbrace{a\frac{\partial\psi}{\partial x}}_{\text{advection}} = \underbrace{\nu\frac{\partial^2\psi}{\partial x^2}}_{\text{diffusion}} - \underbrace{\alpha\psi}_{\text{reaction}}.$$
- solving PDE gives

$$\psi = C\exp(-(\nu k^2 + \alpha + ika)t)\exp(ikx)$$

- length scale $\ell \sim 1/k$; time scale $\tau \sim ((\nu k^2 + \alpha)^2 + k^2 a^2)^{-1/2}$
- small ℓ, $\tau \sim \ell^2/\nu$;   large ℓ, $\tau \sim 1/\alpha$
- Length scale fully coupled to time scale:

$$\tau \sim \frac{\ell^2}{\nu}\left(1 - \ell^2\left(\frac{\alpha}{\nu} + \frac{a^2}{2\nu^2}\right) + \ldots\right)$$

- local fast reaction induces high k, small ℓ, and small τ.

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

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

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

$$\dot{\omega}_i = \sum_{j=1}^{J} \nu_{ij} a_j T^{\beta_j} \exp\left(\frac{-\overline{E}_j}{\overline{R}T} \right) \left(\prod_{k=1}^{N} \overline{\rho}_k^{\nu'_{kj}} \right) \left(1 - \frac{1}{K_{c,j}} \prod_{k=1}^{N} \overline{\rho}_k^{\nu_{kj}} \right)$$

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

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

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

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

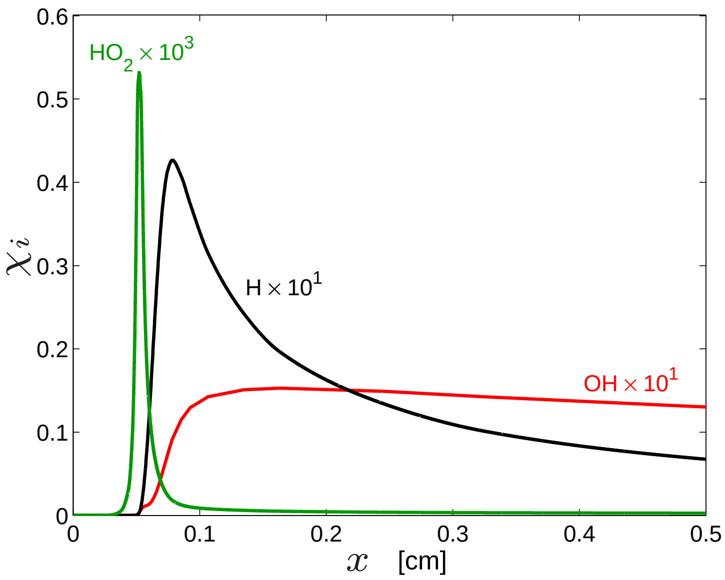
Results

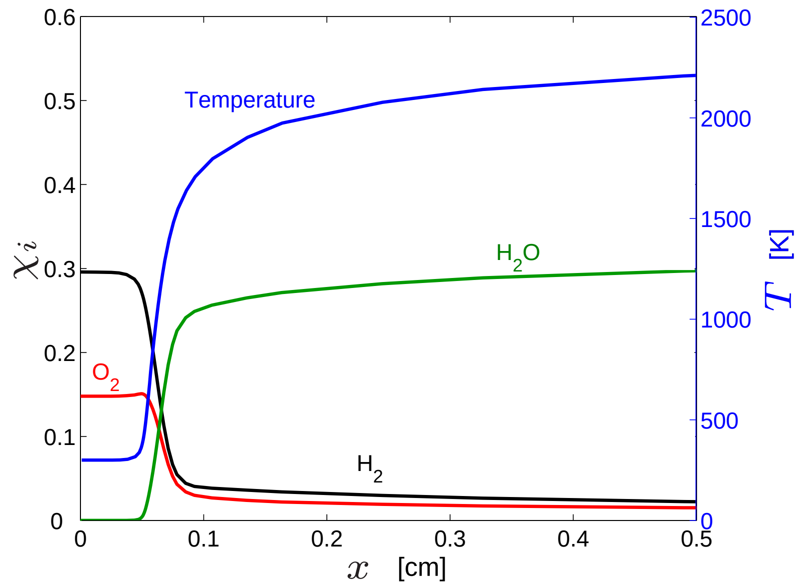
Steady Laminar Premixed Hydrogen-Air Flame

- $N = 9$ 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

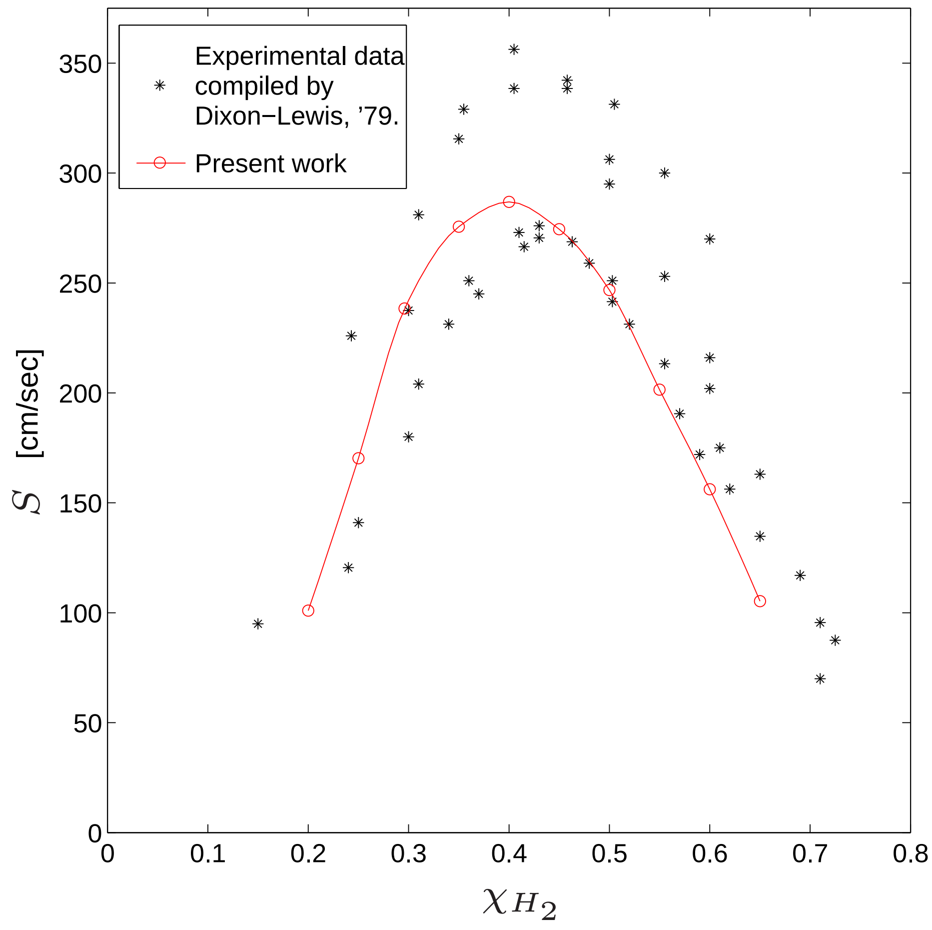
- Good "picture norm" agreement with Smooke *et al.*, '83.





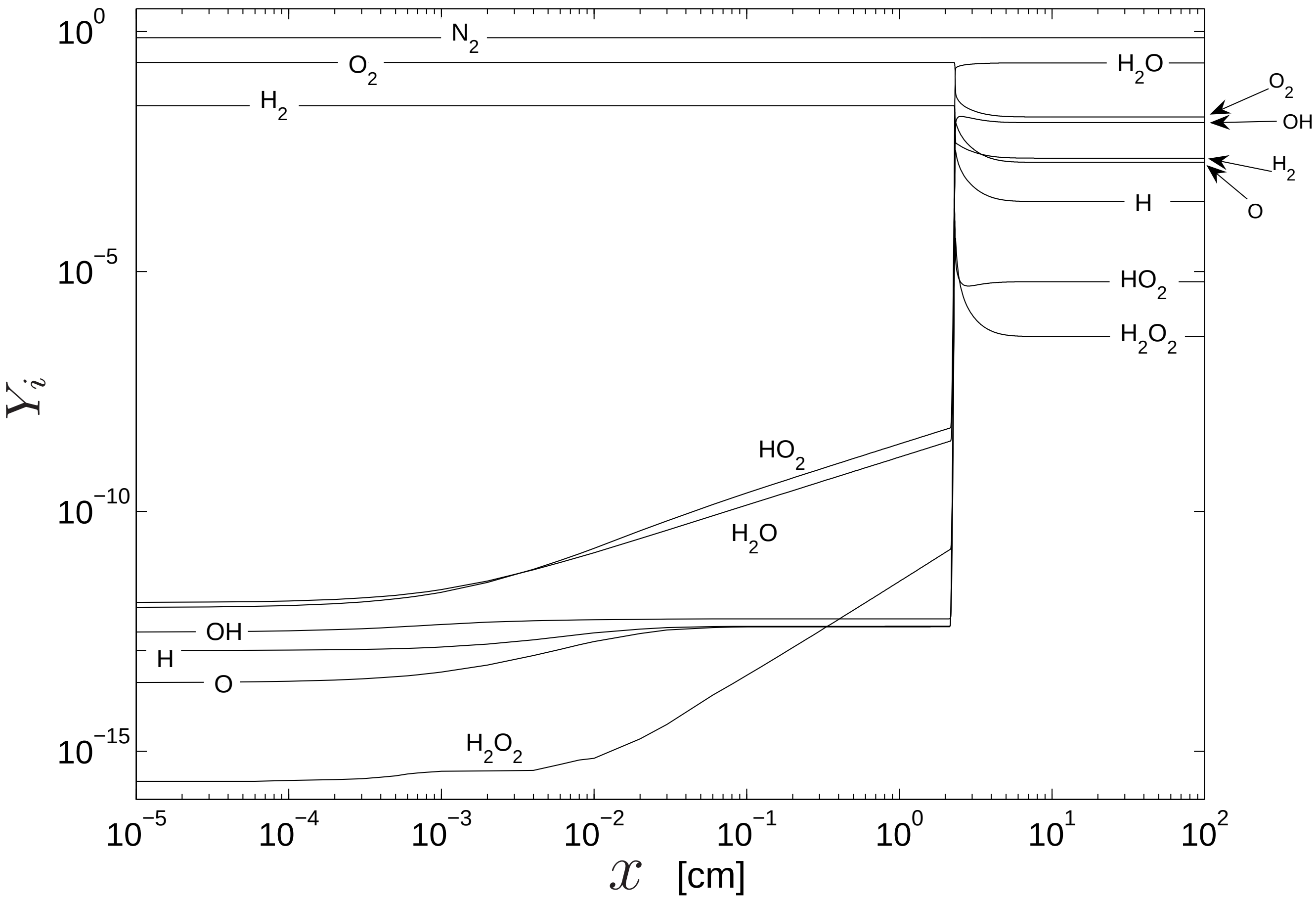
Macro-Experimental Validation

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



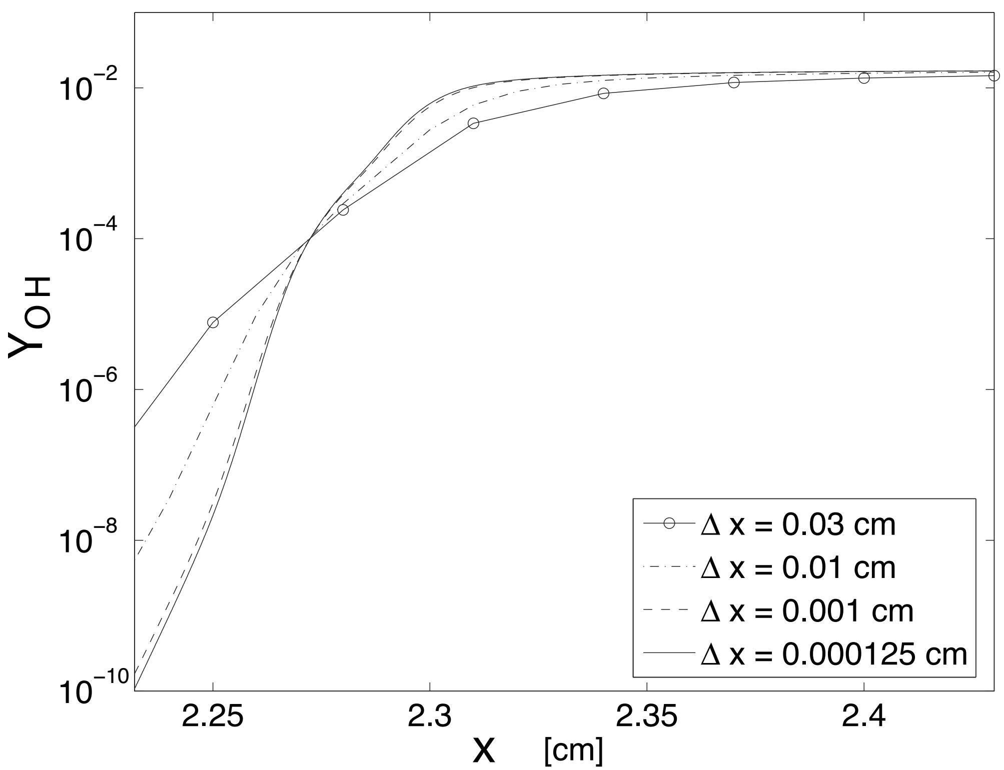
Micro-verification: log-log plot reveals structure at $\mathcal{O}(10^{-4}\ cm)$

- mass fractions versus distance

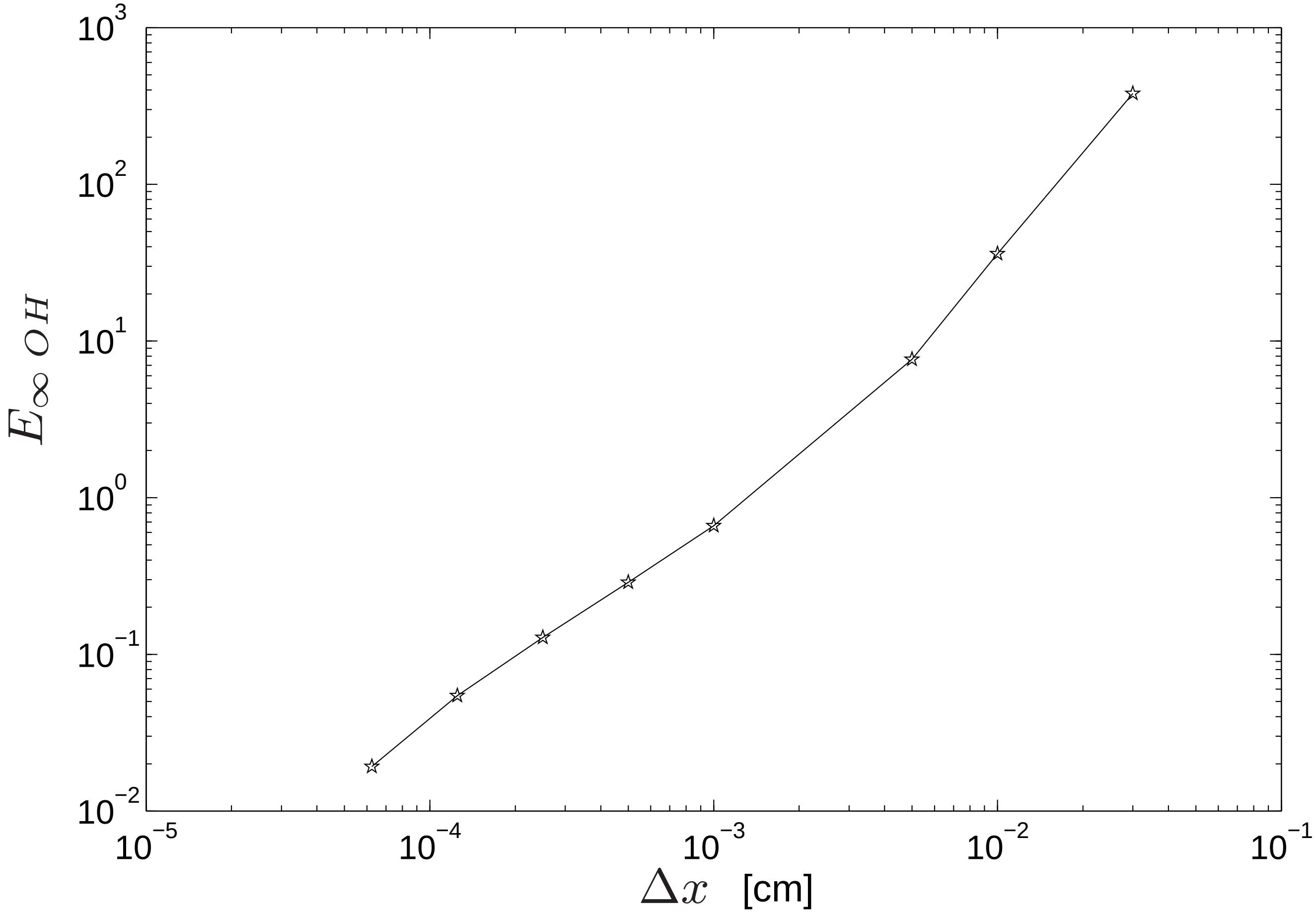


Variation of grid shows physical scales are at $\mathcal{O}(10^{-4}\ cm)$

- 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 $\mathcal{O}(10^{-4}\ cm)$



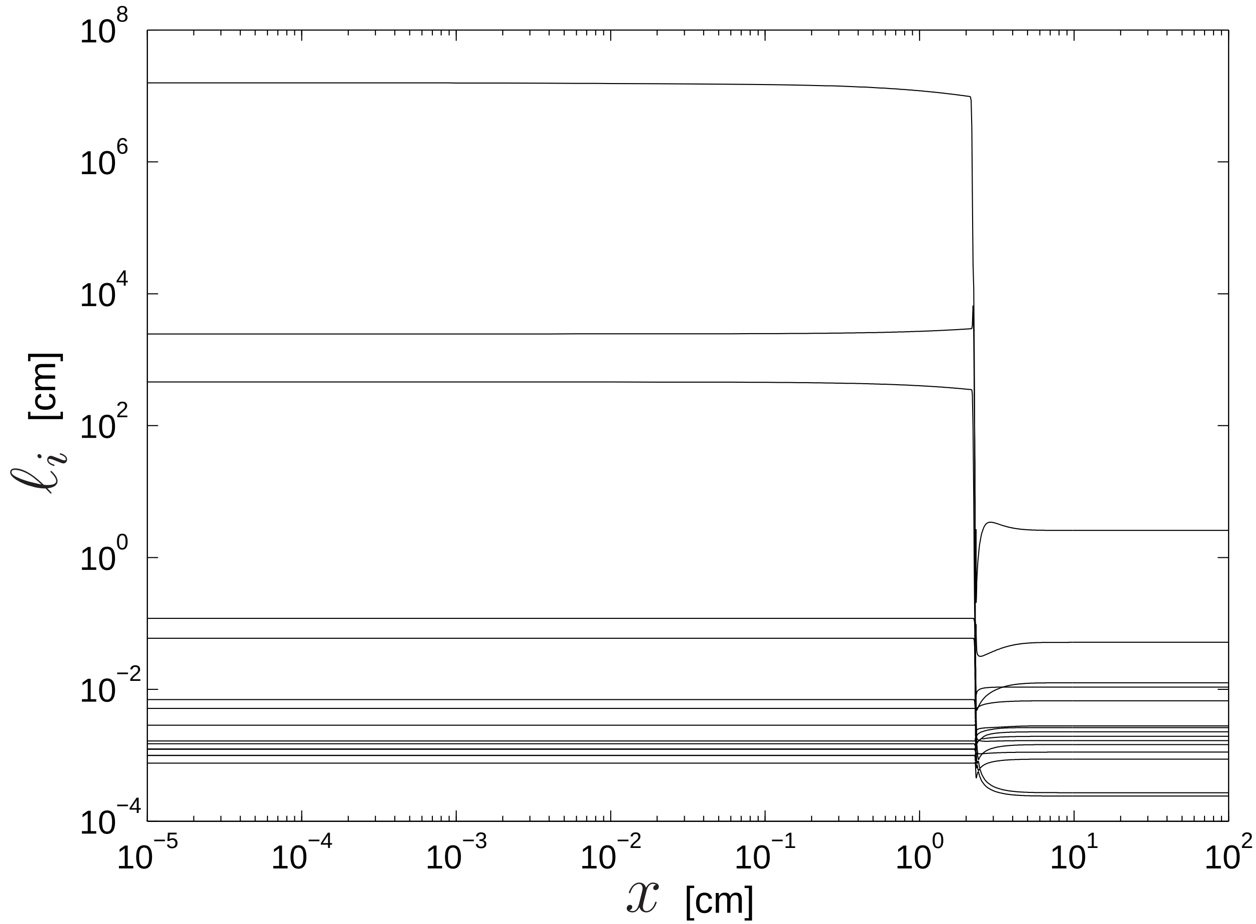
Calculations here are done on a uniform grid

AMR strategy shows physical scales are at $\mathcal{O}(10^{-4}\ cm)$

- `PREMIX` algorithm has an adaptive mesh refinement option for steady laminar one-dimensional flames
- Using common error-control criteria, the algorithm selects a finest grid of $6 \times 10^{-5}\ cm$ for an $H_2 - air$ flame at $1\ atm$.

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

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



Temporal eigenvalue analysis estimates scales are $\mathcal{O}(10^{-4}\ cm)$

- Link between space and time scales in steady flames given by advection time of a Lagrangian particle through the reaction zone.

- Simple time scale estimate found from temporal eigenvalues of spatially homogeneous problem $d\mathbf{z}/dt = \mathbf{f}(\mathbf{z})$ shows $\tau_{finest} \sim 3 \times 10^{-7}\ s$ in induction zone.

- Product of flame speed and finest time scale estimates the finest length scale:

$$\ell_{finest} \sim S\tau_{finest}$$

$$\ell_{finest} \sim (200\ cm/s)(3 \times 10^{-7}\ s) = 6 \times 10^{-5}\ cm$$

$$\ell_{finest} = \mathcal{O}(10^{-4}\ cm)$$

Mean-Free-Path Estimate

- Mean-free-path scale is the cutoff *minimum* length scale associated with continuum theories.

- Simple estimate given by Vincenti and Kruger, 1965:

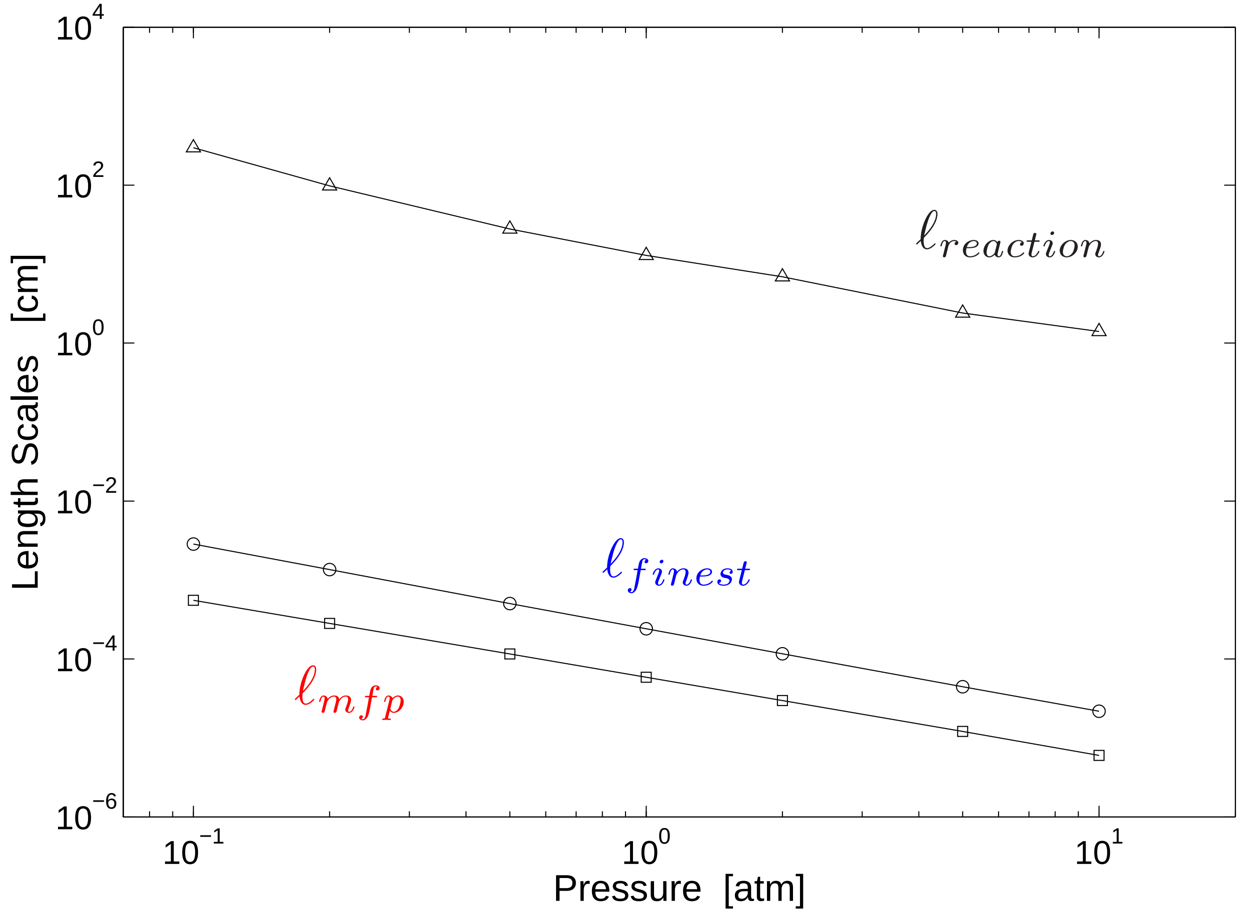
$$\ell_{mfp} = \frac{M}{\sqrt{2}\mathcal{N}\pi d^2 \rho}.$$

- Continuum theory linearized near equilibrium reveals *analytically* that continuum length scales are correlated with mean free path:

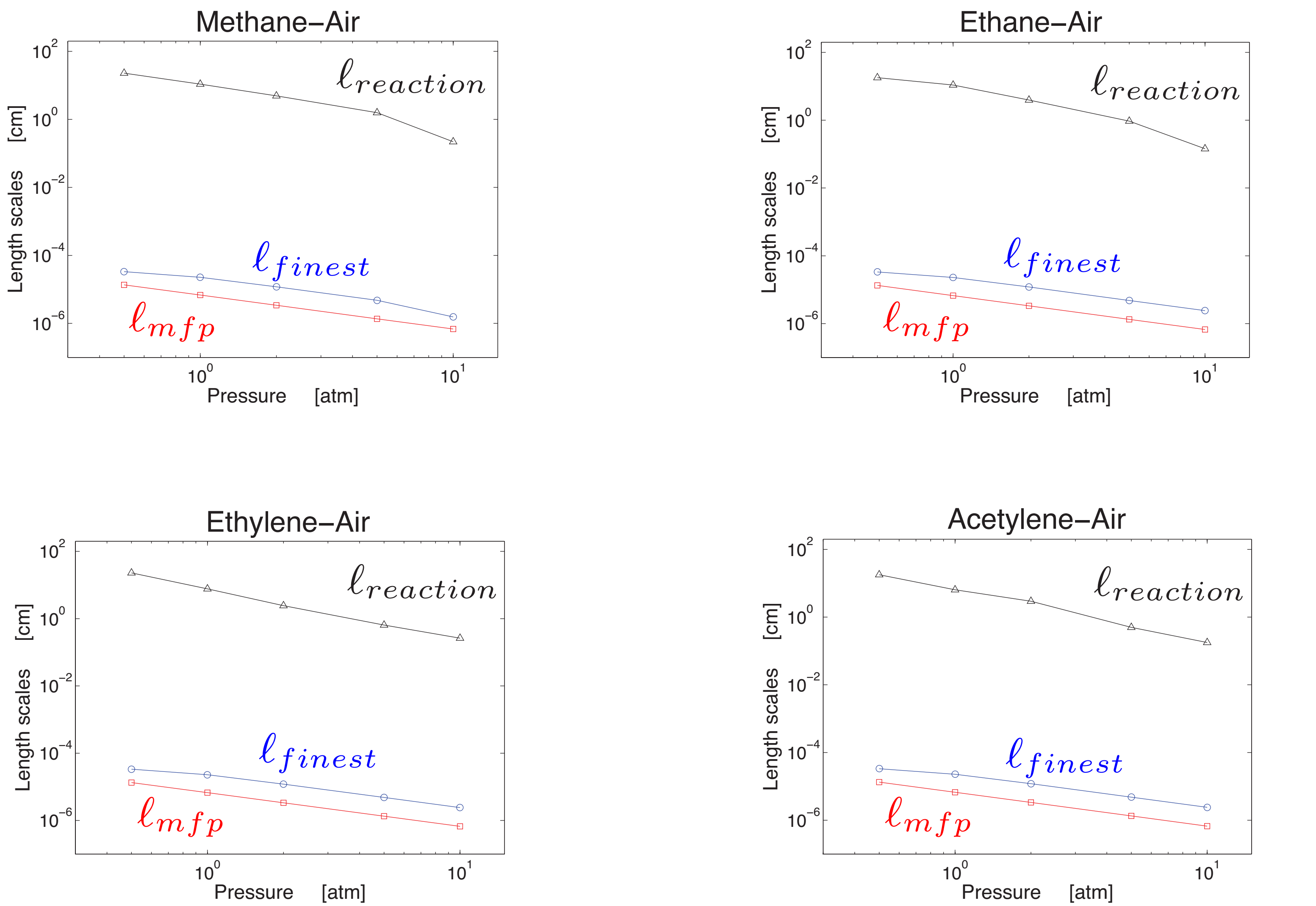
$$\ell_{finest} \approx \ell_{mfp} \underbrace{\left(\frac{8\sqrt{\pi} e^{\frac{E}{\Re T}} \sqrt{K_{eq}} \rho S}{(16\overline{\rho}_{O_2 i} + 8\overline{\rho}_{Oi})^{3/2} \mathcal{N} \sqrt{kTm}} \right)}_{=O(1)}$$

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

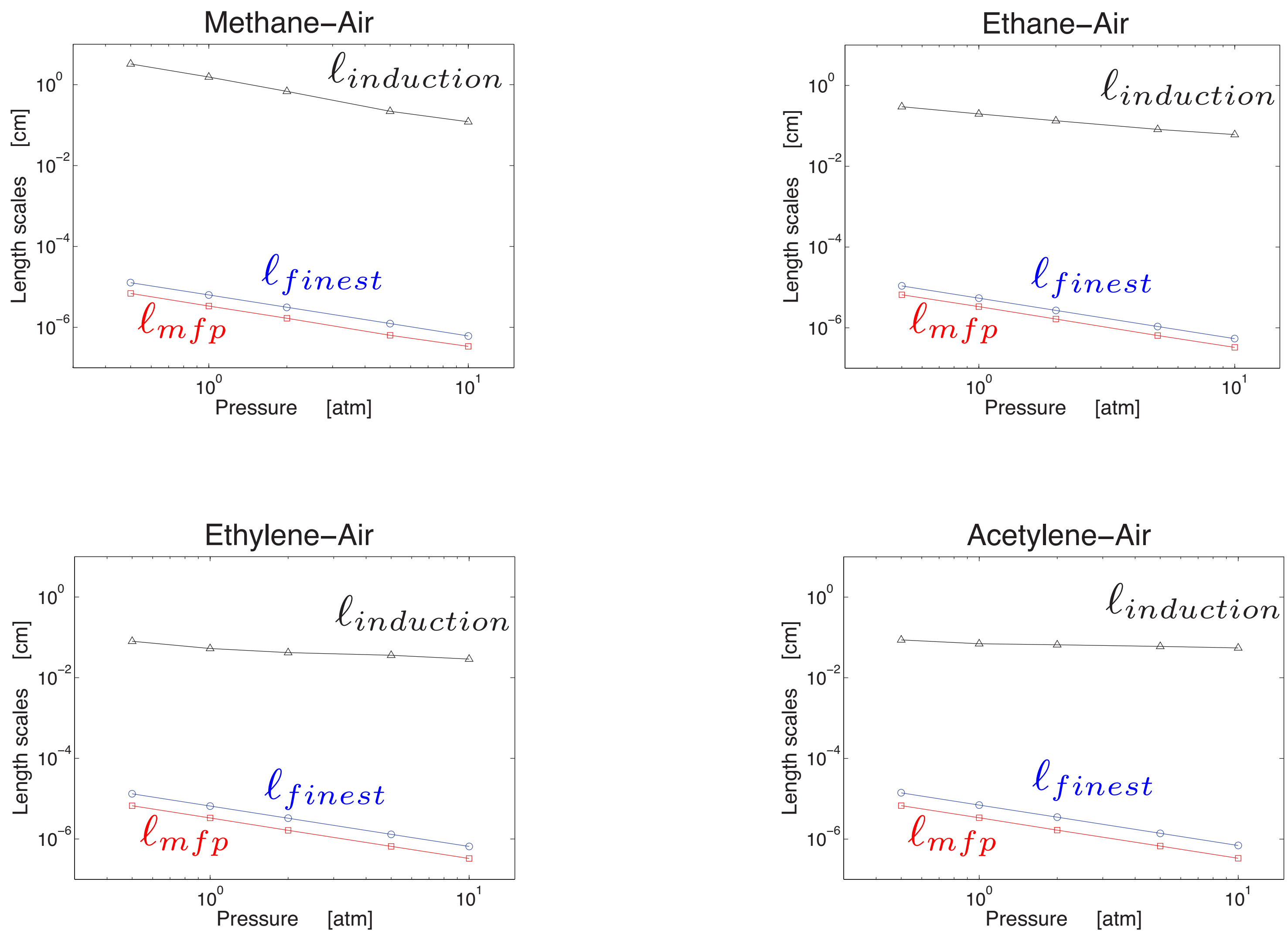
- $\ell_{mfp} = \frac{M}{\sqrt{2}\mathcal{N}\pi d^2\rho}$, the cutoff scale for continuum theory.



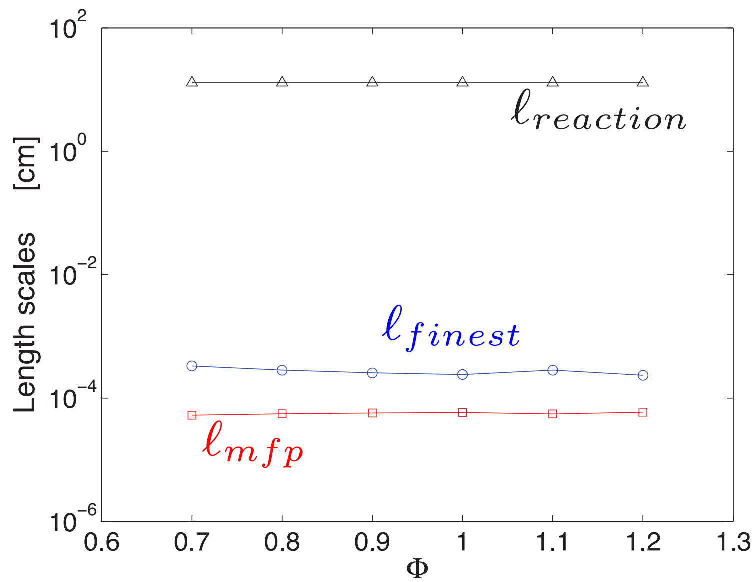
Hydrocarbon deflagration has scales at $\mathcal{O}(10^{-4}\ cm)$



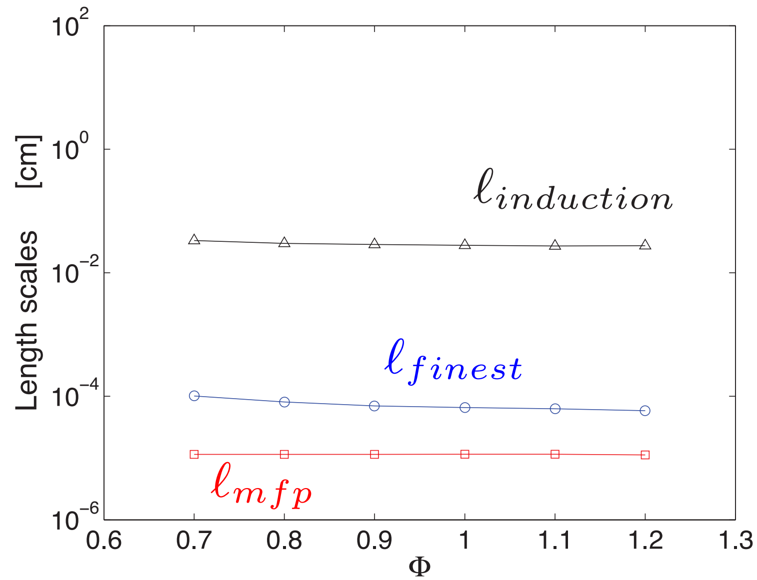
Hydrocarbon detonation has scales at $\mathcal{O}(10^{-4}\ cm)$



Variable equivalence ratio gives scales at $\mathcal{O}(10^{-4}\ cm)$



(a) Laminar premixed flame



(b) Chapman-Jouguet detonation

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

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 the paradigm problem, inert limit

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

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

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

- To solve for the steady structure

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

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

  – 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 species concentrations in 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.