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

• To show such a continuum model can be macro-validated by comparing predictions of flames speeds to observations, while noting $10^{-4} \text{ cm}$-scale structures are too fine for present-day diagnostics.
Scale Coupling in Paradigm Linear System

\( \frac{\partial \psi}{\partial t} + a \frac{\partial \psi}{\partial x} = \nu \frac{\partial^2 \psi}{\partial x^2} - \alpha \psi. \)

- solving PDE gives
  \[ \psi = C \exp\left(-\left(\nu k^2 + \alpha + ika\right)t\right) \exp(ikx) \]

- length scale \( \ell \sim 1/k; \) time scale \( \tau \sim \left((\nu k^2 + \alpha)^2 + k^2 a^2\right)^{-1/2} \)
- small \( \ell, \tau \sim \ell^2/\nu; \) large \( \ell, \tau \sim 1/\alpha \)
- 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 \( \ell, \) and small \( \tau. \)
Mathematical Model

Governing Equations

\[
\frac{\partial \rho}{\partial \tilde{t}} = -\frac{\partial}{\partial \tilde{x}} (\rho \tilde{u}),
\]

\[
\frac{\partial}{\partial \tilde{t}} (\rho \tilde{u}) = -\frac{\partial}{\partial \tilde{x}} (\rho \tilde{u}^2 + p - \tau),
\]

\[
\frac{\partial}{\partial \tilde{t}} \left( \rho \left( e + \frac{\tilde{u}^2}{2} \right) \right) = -\frac{\partial}{\partial \tilde{x}} \left( \rho \tilde{u} \left( e + \frac{\tilde{u}^2}{2} + \frac{p}{\rho} - \frac{\tau}{\rho} \right) + J^q \right),
\]

\[
\frac{\partial}{\partial \tilde{t}} (\rho Y_i) = -\frac{\partial}{\partial \tilde{x}} (\rho \tilde{u} Y_i + J^m_i) + \omega_i M_i, \quad i = 1, \ldots, N - 1.
\]
Constitutive Relations

\[ J^m_i = \rho \sum_{k=1 \atop k \neq i}^N \frac{M_i D_{ik} Y_k}{M} \left( \frac{1}{\chi_k} \frac{\partial \chi_k}{\partial \tilde{x}} + \left( 1 - \frac{M_k}{M} \right) \frac{1}{p} \frac{\partial p}{\partial \tilde{x}} \right) - D^T_i \frac{1}{T} \frac{\partial T}{\partial \tilde{x}}, \]

\[ J^q = q + \sum_{i=1}^N J^m_i h_i - \mathcal{R} T \sum_{i=1}^N \frac{D^T_i}{M_i} \left( \frac{1}{\chi_i} \frac{\partial \chi_i}{\partial \tilde{x}} + \left( 1 - \frac{M_i}{M} \right) \frac{1}{p} \frac{\partial p}{\partial \tilde{x}} \right), \]

\[ \dot{\omega}_i = \sum_{j=1}^J \nu_{ij} a_j T^{\beta_j} \exp \left( \frac{-E_j}{RT} \right) \left( \prod_{k=1}^N \bar{\rho}_k^{\nu_{k,j}} \right) \left( 1 - \frac{1}{K_{c,j}} \prod_{k=1}^N \bar{\rho}_k^{\nu_{k,j}} \right), \]

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

\[ p = \mathcal{R} T \sum_{i=1}^N \frac{\rho Y_i}{M_i}, \]

and others . . .
Dynamical System Formulation

- PDEs $\rightarrow$ ODEs

\[
\frac{d}{dx} (\rho u) = 0, \\
\frac{d}{dx} (\rho uh + J^q) = 0, \\
\frac{d}{dx} (\rho uY^e_l + J^e_l) = 0, \quad l = 1, \ldots, L - 1, \\
\frac{d}{dx} (\rho uY^e_i + J^m_i) = \dot{\omega}_i M_i, \quad i = 1, \ldots, N - L.
\]

- ODEs $\rightarrow$ DAEs

\[A(z) \cdot \frac{dz}{dx} = f(z).\]
Results

Steady Laminar Premixed Hydrogen-Air Flame

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

![Graph showing flame speed data comparison](image-url)
Micro-verification: log-log plot reveals structure at $O(10^{-4} \, \text{cm})$

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

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

![Graph showing the variation of $Y_{OH}$ with different grid increments](image)
Grid convergence shows physical scales are at $O(10^{-4} \text{ cm})$.

Calculations here are done on a uniform grid.
AMR strategy shows physical scales are at $O(10^{-4}\, cm)$

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

- Found from generalized eigenvalues of $A(z) \cdot \frac{dz}{dx} = f(z)$.
Temporal eigenvalue analysis estimates scales are $\mathcal{O}(10^{-4} \text{ cm})$

- 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 \( \frac{dz}{dt} = f(z) \) shows $\tau_{\text{finest}} \sim 3 \times 10^{-7} \text{ s}$ in induction zone.

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

\[
\ell_{\text{finest}} \sim S\tau_{\text{finest}}
\]

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

\[
\ell_{\text{finest}} = \mathcal{O}(10^{-4} \text{ cm})
\]
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:
  \[ \ell_{mfp} = \frac{M}{\sqrt{2N\pi d^2\rho}}. \]

- Continuum theory linearized near equilibrium reveals analytically that continuum length scales are correlated with mean free path:
  \[ \ell_{\text{finest}} \approx \ell_{mfp} \left( \frac{8\sqrt{\pi} E^{\frac{E}{8T}} \sqrt{K_{eq}\rho S}}{(16\rho_{O2i} + 8\rho_{Oi})^{3/2}N\sqrt{kTm}} \right) = O(1) \]
Mean free path estimates shows scales are $\mathcal{O}(10^{-4} \text{ cm})$

- $\ell_{mfp} = \frac{M}{\sqrt{2N\pi d^2 \rho}}$, the cutoff scale for continuum theory.
Hydrocarbon deflagration has scales at $\mathcal{O}(10^{-4} \text{ cm})$.
Hydrocarbon detonation has scales at $\mathcal{O}(10^{-4} \text{ cm})$.
Variable equivalence ratio gives scales at $\mathcal{O}(10^{-4}\, \text{cm})$

(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...”

## Comparison with Other Published Results

<table>
<thead>
<tr>
<th>Ref.</th>
<th>Mixture molar ratio</th>
<th>$\Delta x, (cm)$</th>
<th>$\ell_{\text{finest}}, (cm)$</th>
<th>$\ell_{mfp}, (cm)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1.26H_2 + O_2 + 3.76N_2$</td>
<td>$2.50 \times 10^{-2}$</td>
<td>$8.05 \times 10^{-4}$</td>
<td>$4.33 \times 10^{-5}$</td>
</tr>
<tr>
<td>2</td>
<td>$CH_4 + 2O_2 + 10N_2$</td>
<td>unknown</td>
<td>$6.12 \times 10^{-4}$</td>
<td>$4.33 \times 10^{-5}$</td>
</tr>
<tr>
<td>3</td>
<td>$0.59H_2 + O_2 + 3.76N_2$</td>
<td>$3.54 \times 10^{-2}$</td>
<td>$4.35 \times 10^{-5}$</td>
<td>$7.84 \times 10^{-6}$</td>
</tr>
<tr>
<td>4</td>
<td>$CH_4 + 2O_2 + 10N_2$</td>
<td>$1.56 \times 10^{-3}$</td>
<td>$2.89 \times 10^{-5}$</td>
<td>$6.68 \times 10^{-6}$</td>
</tr>
</tbody>
</table>


The modified equation for the paradigm problem, inert limit

\[ \frac{\partial \psi}{\partial t} + a \frac{\partial \psi}{\partial x} = \nu \frac{\partial^2 \psi}{\partial x^2}, \]

\[ \frac{\psi_{i+1}^n - \psi_i^n}{\Delta t} + a \frac{\psi_i^n - \psi_{i-1}^n}{\Delta x} = \nu \frac{\psi_{i+1}^n - 2\psi_i^n + \psi_{i-1}^n}{\Delta x^2}, \]

\[ \frac{\partial \psi}{\partial t} + a \frac{\partial \psi}{\partial x} = \left( \nu + \frac{a \Delta x}{2} \left( 1 - \frac{a \Delta t}{\Delta x} \right) \right) \frac{\partial^2 \psi}{\partial x^2} \]

\[ + \frac{a \Delta x^2}{6} \left( -1 + \left( \frac{a \Delta t}{\Delta x} \right)^2 + 6 \frac{\nu \Delta t}{\Delta x^2} \right) \frac{\partial^3 \psi}{\partial x^3} + \ldots \]

- Discretization-based terms alter the dynamics.
- Numerical diffusion could suppress physical instability.
To solve for the steady structure

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

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

- Analogous to what has been done in our work

\[
\lambda = \begin{bmatrix} 0 \\ a/\nu \end{bmatrix},
\]

\( \Rightarrow \ell_{\text{finest}} = \nu/a. \)

- 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.