Accurate Estimates of Fine Scale Reaction Zone Thicknesses in Hydrocarbon Detonations

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Motivation

- Detailed kinetics pervade continuum simulations.
- The finest length scale predicted by continuum models is usually not clarified and often not resolved.
- The relation of finest continuum length scales to mean-free-path scales from collision theory is unclear.
- Tuning computational results to match experiments without first harmonizing with underlying mathematics renders predictions unreliable.

Computations Can Fail

Attempts to computationally *pre-dict*, not post-dict, results of a benchmark high speed combustion experiment with ram accelerators generated “widely different outcomes.”

LeBlanc, et al., *J. Physique IV*, 2000.

Why does this happen? Poor numerical resolution of physical structures?

Verification and Validation

- *Verification*: solving the equations right (mathematics)
- *Validation*: solving the right equations (physics)
- Verification must precede validation; both must be done to avoid failure.
- To assess any mathematical model's viability, its predictions must not be strong functions of the discrete algorithm used in obtaining an approximate solution.
- See work of Roache or Oberkampf.

AIAA Policy Statement of Numerical Accuracy, 2005

“The AIAA journals will not accept for publication any paper reporting numerical solutions of an engineering problem that fails adequately to address the accuracy of the computed results...The accuracy of the computed results is concerned with how well the specified governing equations in the paper have been solved numerically. The appropriateness of the governing equations for modeling the physical phenomena and comparison with experimental data is not part of this evaluation. ”

Literature Review for Methane Detonation

- Westbrook, *et al.*, *Comb. Flame*, 1991.
- Yungster and Rabinowitz, *J. Propul. Power*, 1994.
- Petersen and Hanson, *J. Propul. Power*, 1999.
- Hanson, *et al.*, *J. Propul. Power*, 2000.
- Jeung, *et al.*, *Appl. Num. Math.*, 2001.
- Powers and Paolucci, *AIAA J.*, 2005 (H_2-air).
- Powers, *J. Propul. Power*, 2006 (multi-scale).

Continuum Model: Reactive Euler Equations

- one-dimensional,
- steady,
- inviscid,
- detailed Arrhenius kinetics,
- Troe formalism for pressure-dependent rates,
- calorically imperfect ideal gas mixture.

Continuum Model: Reactive Euler Equations

$$\begin{aligned}
\rho u &= \rho_o D, \\
\rho u^2 + p &= \rho_o D^2 + p_o, \\
e + \frac{u^2}{2} + \frac{p}{\rho} &= e_o + \frac{D^2}{2} + \frac{p_o}{\rho_o}, \\
\frac{dY_i}{dx} &= f_i \equiv \frac{\dot{\omega}_i M_i}{\rho_o D}.
\end{aligned}$$

Supplemented by EOS and law of mass action.

Reduced Model

Algebraic reductions lead to a final form of

$$\frac{dY_i}{dx} = f_i(Y_1, \ldots, Y_{N-L}),$$

with

- N: number of molecular species
- L: number of atomic elements

Eigenvalue Analysis of Local Length Scales

Local behavior is modeled by

$$\frac{d\mathbf{Y}}{dx} = \mathbf{J} \cdot (\mathbf{Y} - \mathbf{Y}^*) + \mathbf{b}, \qquad \mathbf{Y}(x^*) = \mathbf{Y}^*.$$

whose solution is

$$\mathbf{Y}(x) = \mathbf{Y}^* + \left(\mathbf{P} \cdot e^{\mathbf{\Lambda}(x-x^*)} \cdot \mathbf{P}^{-1} - \mathbf{I}\right) \cdot \mathbf{J}^{-1} \cdot \mathbf{b}.$$

Here, $\mathbf{\Lambda}$ has eigenvalues λ_i of Jacobian $\mathbf{J}$ in its diagonal.

Length scales given by

$$\ell_i(x) = \frac{1}{|\lambda_i(x)|}.$$

Computational Methods

- A standard ODE solver (DLSODE) was used to integrate the equations.
- Standard IMSL subroutines were used to evaluate the local Jacobians and eigenvalues at every step.
- The CHEMKIN software package was used to evaluate kinetic rates and thermodynamic properties.
- Computation time was typically three minutes on a $1\,GHz$ HP Linux machine.

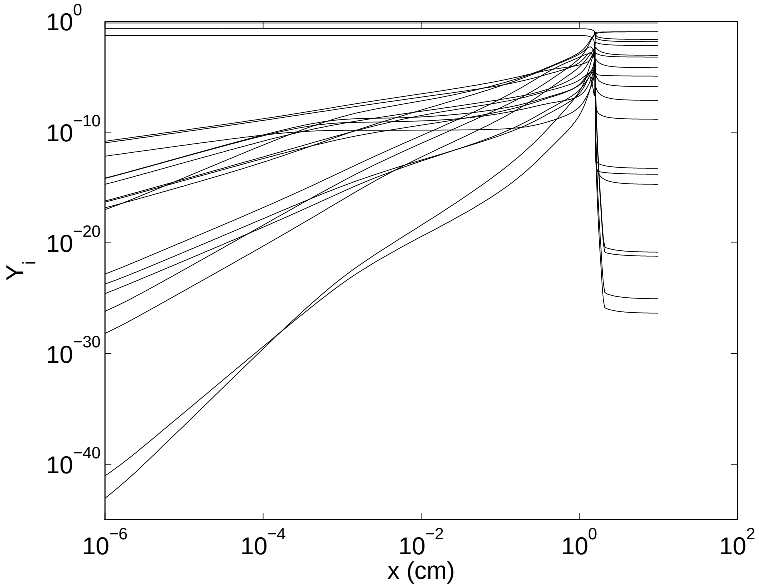
Physical System

- CJ methane-air detonation: $CH_4 + 2O_2 + 7.52N_2$.
- $N = 21$ species, $J = 52$ reversible reactions.
- Based on model of Yungster and Rabinowitz, 1994.
- Troe formalism for pressure-dependency from GRI 3.0.
- $p_o = 1\,atm, T_o = 298\;K$, $M_{CJ} = 5.13$.
- For scientific reproducibility, full exposition of thermochemistry given in paper.

Verification and Validation of Detailed Kinetics Model

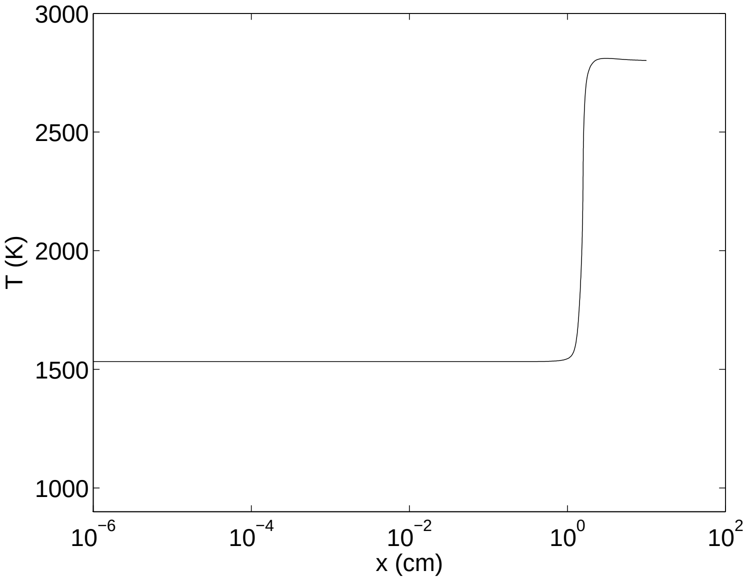
- *Mathematical verification*: predicts similar ignition delay time as calculations of Petersen and Hanson: $30\,\mu s$ vs. $25\,\mu s$ at $T_o = 1500\,K$, $p_o = 150\,atm$.
- *Experimental validation*: predicts ignition delay time observations of Spadaccini and Colket: $115\,\mu s$ vs. $139\,\mu s$ at $T_o = 1705\,K$, $p_o = 6.6\,atm$.

Mass Fractions versus Distance



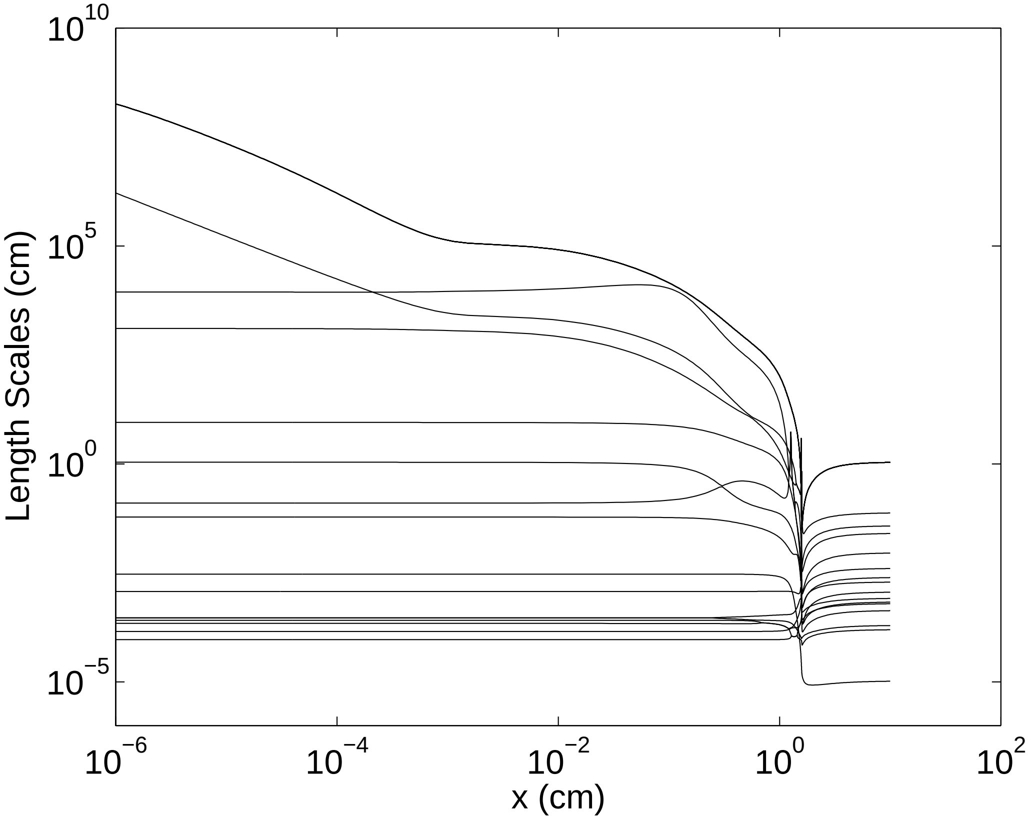
- significant evolution at fine length scales $x \sim 10^{-4}\ cm$.
- CJ state and induction zone length agree with Westbrook and many others.

Temperature Profile



- Temperature flat in the post-shock induction zone $0 < x < 1.5\, cm$.
- Thermal explosion followed by relaxation to equilibrium at $x \sim 10\, cm$.

Eigenvalue Analysis: Length Scale Evolution



Finest length scale is $10^{-5}\ cm$.

Continuum versus Collision Theory

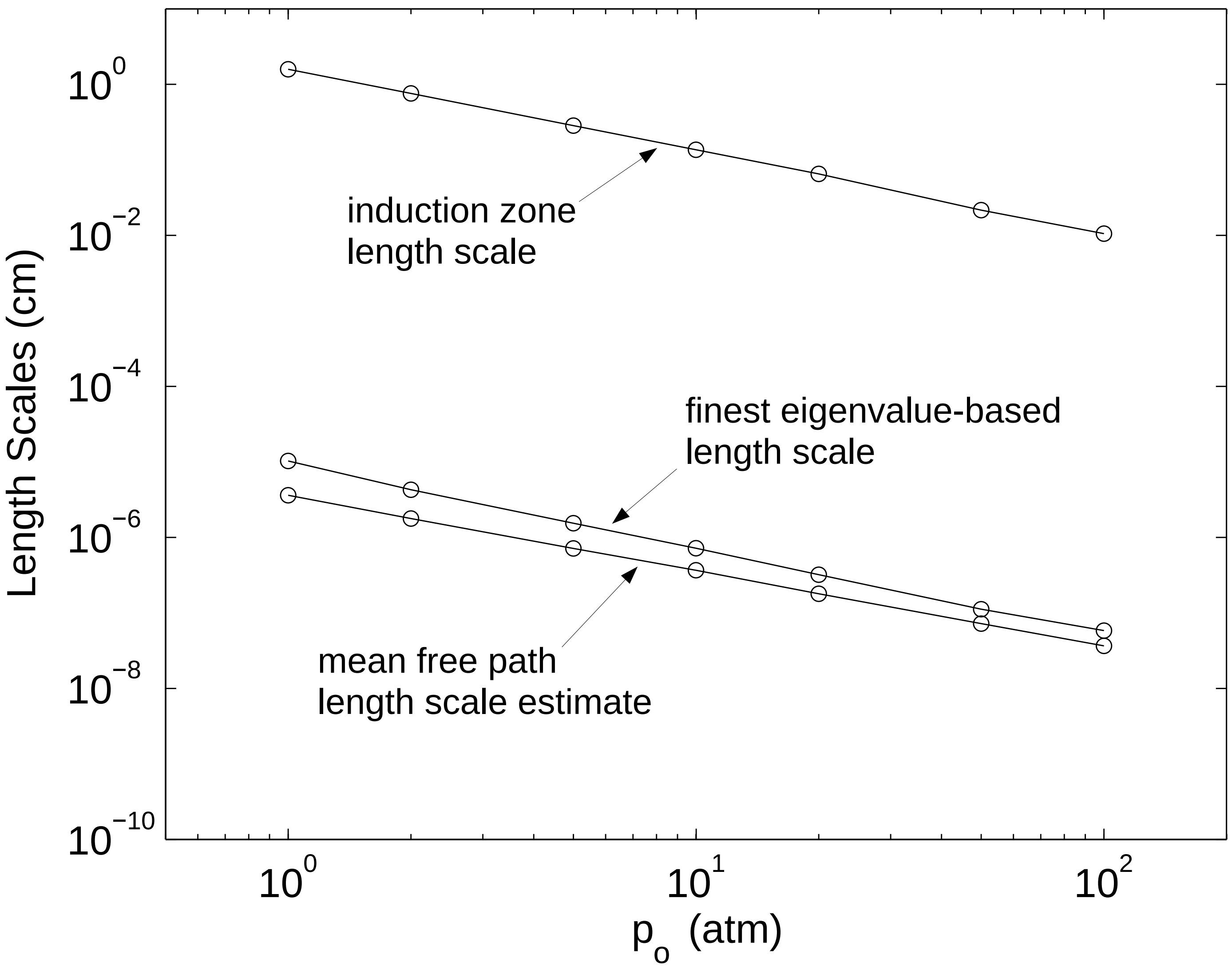
- Continuum theory: averaged collision theory:

$$A_j \sim 2\mathsf{N}\mathsf{d}^2\sqrt{\frac{2\pi\mathsf{k}}{\mathsf{m}}} = 7.24 \times 10^{12}\ \frac{cm^3}{mole\ s\ K^{1/2}}$$

- continuum theory valid at or above mean free path length scale:

$$\ell_{mfp} \sim \frac{\mathsf{m}}{\sqrt{2}\pi\mathsf{d}^2\rho} \sim 10^{-5}\ cm$$

Continuum versus Collision Theory



Recently Published Results for Strongly Overdriven Detonations in Methane-Air

Ref.	$\ell_{ind}\ (cm)$	$\ell_f\ (cm)$	$\Delta x\ (cm)$	$\Delta x/\ell_f$
Yungster, *et al.*, 1994	3.6×10^{-2}	1.8×10^{-6}	1.4×10^{-2}	7000
Jameson, *et al.*, 1998	3.8×10^{-2}	1.9×10^{-6}	2.1×10^{-4}	110
Jeung, *et al.*, 2001	3.7×10^{-2}	1.9×10^{-6}	2.7×10^{-4}	142
Hanson, *et al.*, 2000	3.6×10^{-2}	1.8×10^{-6}	2.8×10^{-4}	155
Parra-Santos, *et al.*, 2005	2.6×10^{-2}	1.2×10^{-5}	$-$	$-$

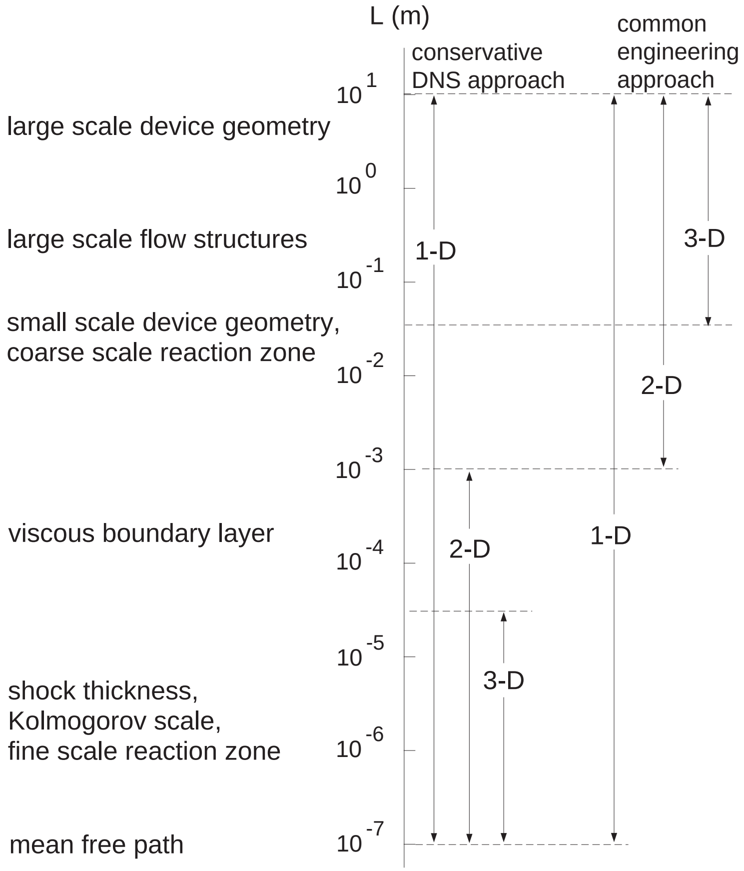
All induction zones are resolved.

All finest scales are severely under-resolved.

What does this all mean?

- Leblanc, *et al*, *J. Physique IV*, 2000, show computations predicting *“widely different outcomes”* which are sensitive to induction zone dynamics in attempting to reproduce results of benchmark ram accelerator experiment.
- Tangirala, *et al.*, *CST*, 2004, find DDT in pulse detonation engine to be *“underpredicted”* by computations.
- Lack of resolution may explain the discrepancies; however, resolution is necessary in any case.

Estimate of Present Computational Capability



Conclusions

- For repeatable scientific calculation, the finest physical scales intrinsic to the model must be resolved, whatever the model.
- Length scale estimates of $10^{-5}\ cm$ for methane-air detonation are nearly identical to previous hydrogen-air estimates as well those of underlying molecular collision theory.
- Collision-based continuum models with detailed kinetics must be resolved down to the mean free path for DNS.
- We encourage creation of a widely accessible and maintained thermochemistry data base to assure full scientific reproducibility to limit size of publications.