Resolution Matters: Issues in Computational Simulation of Detailed Kinetics Gas Phase Combustion

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58th Annual Meeting of the APS DFD

Chicago, Illinois; 20 November 2005

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Motivation

- Detailed kinetics models are widely used in detonation simulations.
- The finest length scale predicted by such models is usually not clarified and often not resolved.
- Tuning computational results to match experiments without first harmonizing with underlying mathematics renders predictions unreliable.
- See Powers and Paolucci, *AIAA Journal*, 2005.

Model: Steady 1D Reactive Euler Equations

$$\rho u = \rho_o D,$$

$$\rho u^2 + p = \rho_o D^2 + p_o,$$

$$e + \frac{u^2}{2} + \frac{p}{\rho} = e_o + \frac{D^2}{2} + \frac{p_o}{\rho_o},$$

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

$$e = \sum_{i=1}^{N} Y_i \left(h_{i,f}^o + \int_{T_o}^{T} c_{pi}(\hat{T})\, d\hat{T} - \frac{\Re T}{M_i} \right),$$

$$\frac{dY_i}{dx} = \frac{M_i}{\rho_o D} \sum_{j=1}^{J} \nu_{ij} \alpha_j T^{\beta_j} e^{\left(\frac{-E_j}{\Re T}\right)} \left(\underbrace{\prod_{k=1}^{N} \left(\frac{\rho Y_k}{M_k}\right)^{\nu'_{kj}}}_{\text{forward}} - \underbrace{\frac{1}{K_j^c} \prod_{k=1}^{N} \left(\frac{\rho Y_k}{M_k}\right)^{\nu''_{kj}}}_{\text{reverse}} \right)$$

Eigenvalue Analysis of Local Length Scales

Algebraic reduction yields

$$\frac{d\mathbf{Y}}{dx} = \mathbf{f}(\mathbf{Y}).$$

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

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

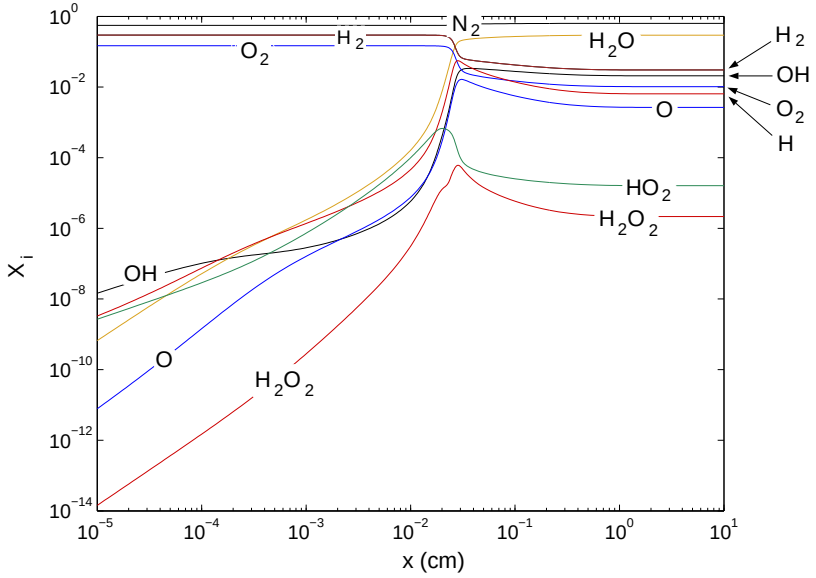
Computational Methods

- 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 one minute on a $1\,GHz$ HP Linux machine.

Physical System

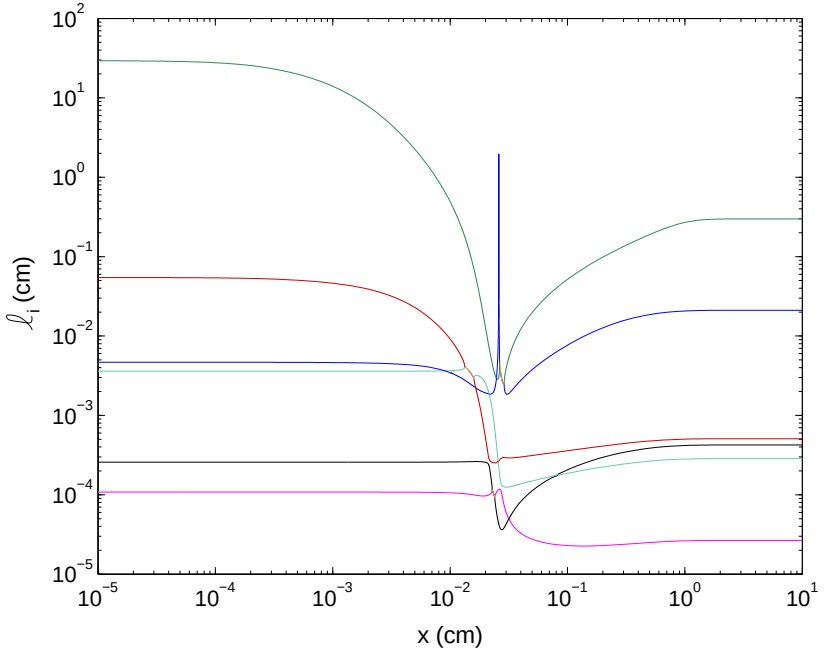
- Hydrogen-air detonation: $2H_2 + O_2 + 3.76N_2$.
- $N = 9$ molecular species, $L = 3$ atomic elements, $J = 19$ reversible reactions.
- $p_o = 1\ atm$.
- $T_o = 298\ K$.
- Identical to system studied by both Shepherd (1986) and Mikolaitis (1987).

Mole Fractions versus Distance



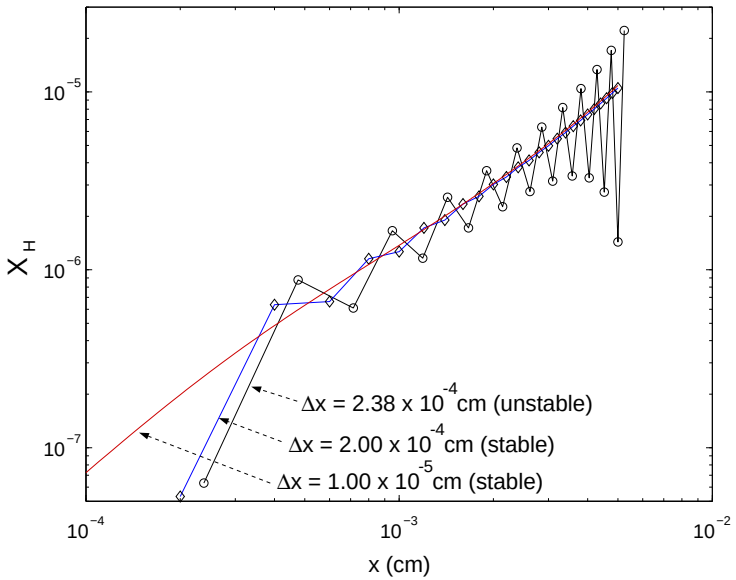
- significant evolution at fine length scales $x < 10^{-3}\ cm$.
- results agree with those of Shepherd.

Eigenvalue Analysis: Length Scale Evolution



- Finest length scale: $2.3 \times 10^{-5}\ cm$.
- Coarsest length scale $3.0 \times 10^{1}\ cm$.
- Finest length scale similar to that necessary for numerical stability of ODE solver.

Numerical Stability



- Discretizations finer than finest physical length scale are numerically stable.
- Discretizations coarser than finest physical length scale are numerically unstable.

Examination of Recently Published Results

Reference	$\ell_{ind}\ (cm)$	$\ell_f\ (cm)$	$\Delta x\ (cm)$	Under-resolution
Oran, *et al.*, 1998	2×10^{-1}	2×10^{-4}	4×10^{-3}	2×10^{1}
Jameson, *et al.*, 1998	2×10^{-2}	5×10^{-5}	3×10^{-3}	6×10^{1}
Hayashi, *et al.*, 2002	2×10^{-2}	1×10^{-5}	5×10^{-4}	5×10^{1}
Hu, *et al.*, 2004	2×10^{-1}	2×10^{-4}	3×10^{-3}	2×10^{1}
Powers, *et al.*, 2001	2×10^{-2}	3×10^{-5}	8×10^{-5}	3×10^{0}
Osher, *et al.*, 1997	2×10^{-2}	3×10^{-5}	3×10^{-2}	1×10^{3}
Merkle, *et al.*, 2002	5×10^{-3}	8×10^{-6}	1×10^{-2}	1×10^{3}
Sislian, *et al.*, 1998	1×10^{-1}	2×10^{-4}	1×10^{0}	5×10^{3}
Jeung, *et al.*, 1998	2×10^{-2}	6×10^{-7}	6×10^{-2}	1×10^{5}

All are under-resolved, some severely.

Conclusions

- Detonation calculations are often under-resolved, by as much as five orders of magnitude.
- Equilibrium properties are insensitive to resolution, while transient phenomena can be sensitive.
- Sensitivity of results to resolution is not known *a priori*.
- Numerical viscosity stabilizes instabilities.
- For a repeatable scientific calculation of detonation, the finest physical scales must be resolved.

Moral

You either do detailed kinetics with the proper resolution,

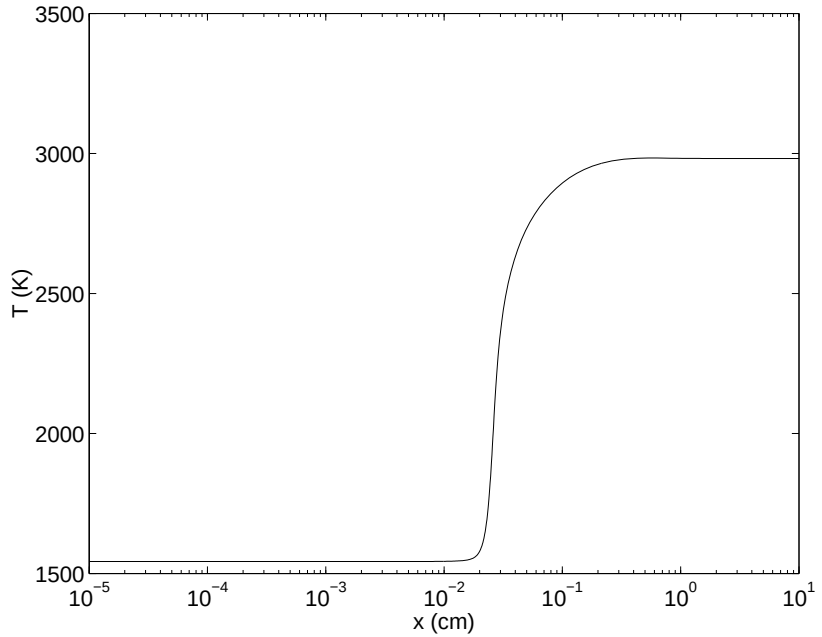
or

you are fooling yourself and others, in which case you should stick with reduced kinetics!

Detailed Kinetics Model

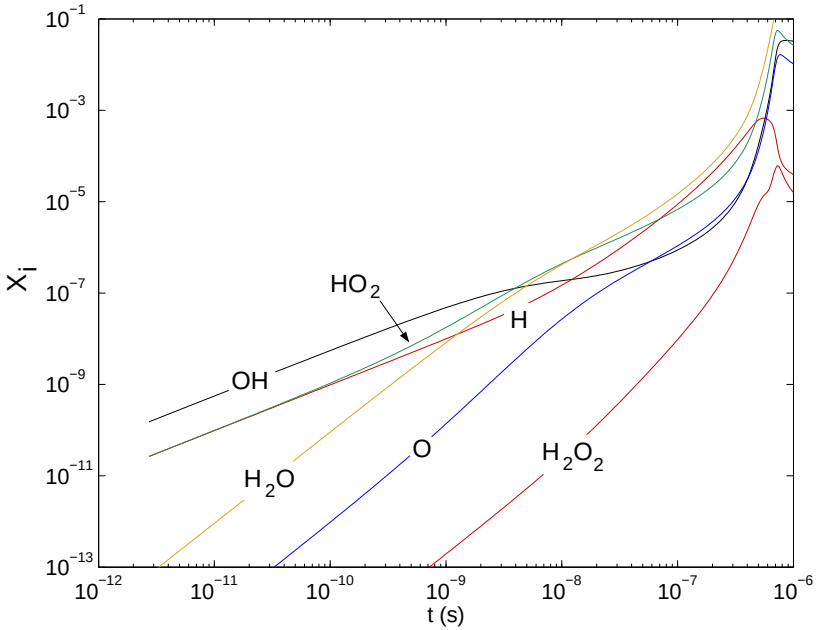
j	Reaction	A_j	β_j	E_j
1	$H_2 + O_2 \rightleftharpoons OH + OH$	1.70×10^{13}	0.00	47780
2	$OH + H_2 \rightleftharpoons H_2O + H$	1.17×10^{9}	1.30	3626
3	$H + O_2 \rightleftharpoons OH + O$	5.13×10^{16}	-0.82	16507
4	$O + H_2 \rightleftharpoons OH + H$	1.80×10^{10}	1.00	8826
5	$H + O_2 + M \rightleftharpoons HO_2 + M$	2.10×10^{18}	-1.00	0
6	$H + O_2 + O_2 \rightleftharpoons HO_2 + O_2$	6.70×10^{19}	-1.42	0
7	$H + O_2 + N_2 \rightleftharpoons HO_2 + N_2$	6.70×10^{19}	-1.42	0
8	$OH + HO_2 \rightleftharpoons H_2O + O_2$	5.00×10^{13}	0.00	1000
9	$H + HO_2 \rightleftharpoons OH + OH$	2.50×10^{14}	0.00	1900
10	$O + HO_2 \rightleftharpoons O_2 + OH$	4.80×10^{13}	0.00	1000
11	$OH + OH \rightleftharpoons O + H_2O$	6.00×10^{8}	1.30	0
12	$H_2 + M \rightleftharpoons H + H + M$	2.23×10^{12}	0.50	92600
13	$O_2 + M \rightleftharpoons O + O + M$	1.85×10^{11}	0.50	95560
14	$H + OH + M \rightleftharpoons H_2O + M$	7.50×10^{23}	-2.60	0
15	$H + HO_2 \rightleftharpoons H_2 + O_2$	2.50×10^{13}	0.00	700
16	$HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$	2.00×10^{12}	0.00	0
17	$H_2O_2 + M \rightleftharpoons OH + OH + M$	1.30×10^{17}	0.00	45500
18	$H_2O_2 + H \rightleftharpoons HO_2 + H_2$	1.60×10^{12}	0.00	3800
19	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$	1.00×10^{13}	0.00	1800

Temperature Profile



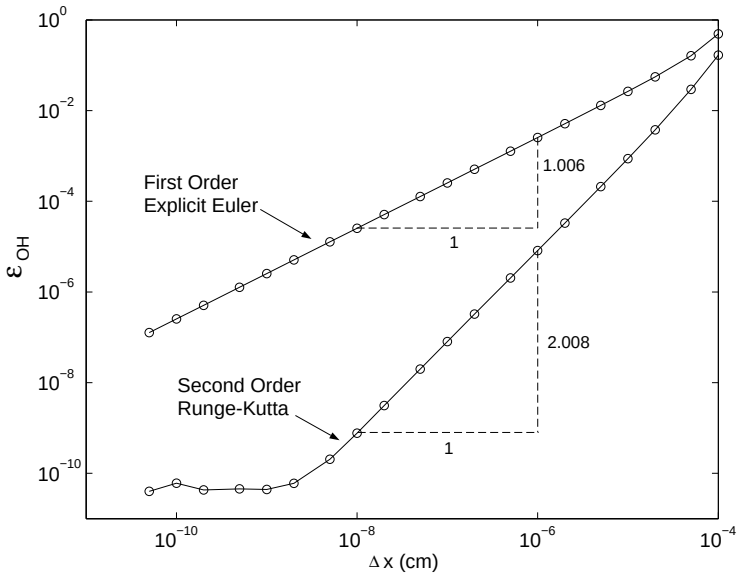
- Temperature flat in the post-shock induction zone $0 < x < 2.6 \times 10^{-2}\ cm$.
- Thermal explosion followed by relaxation to equilibrium at $x \sim 10^{0}\ cm$.

Verification: Comparison with Mikolaitis



- Lagrangian calculation allows direct comparison with Mikolaitis' results.
- agreement very good.

Grid Convergence



- Finest length scale must be resolved to converge at proper order.
- Results are converging at proper order for first and second order discretizations.