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Stability of Flame-Shock Coupling in Detonation Waves: 1D Dynamics

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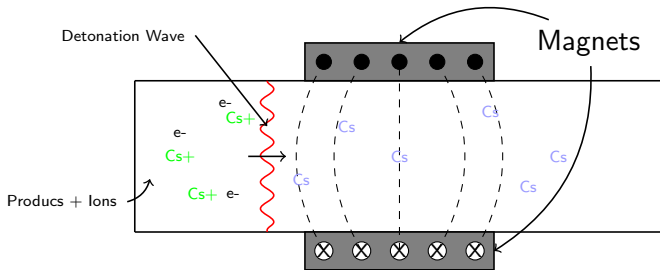
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28 July 2011

Motivation

- How will energy extraction/introduction via joule heating($\vec{J} \cdot \vec{E}$) affect the stability of the detonation?
- How will the magnetic Pressure($\vec{J} \times \vec{B}$) evolution affect the Reaction Zone and detonation stability?



Goals of the Present Study

- In order to understand detonation-magnetic field interactions, one must first understand the stability criteria of an unmagnetized, unsupported detonation.
- Explore the nonlinear dynamics involved in detonation stability
 - ▶ Induction lengths relation to kinetics & dynamics
- Examine the coupling of large and small length scale physics
 - ▶ Correlating different modes of peak pressure behavior to small scale phenomena

Numerical Methodology

Inviscid, one-dimensional Euler equations using multi-step, reversible reaction mechanism:

$$\mathbf{Q}_t + \mathbf{F}(\mathbf{Q})_x = \mathbf{S}(\mathbf{Q}) \quad (1)$$

where the vectors represented by $\mathbf{Q}$, $\mathbf{F}$, and $\mathbf{S}$ are, respectively,

$$\mathbf{Q} = \begin{pmatrix} \rho_s \\ \rho u \\ \hat{E} \end{pmatrix}, \mathbf{F} = \begin{pmatrix} \rho_s u \\ \rho u^2 + P \\ (\hat{E} + P)u \end{pmatrix}, \mathbf{S} = \begin{pmatrix} \omega_s \\ 0 \\ \sum_s \omega_s e_{0s} \end{pmatrix} \quad (2)$$

where the total mixture density $\rho = \sum_s \rho_s$, and the total energy $\hat{E}$ may be written

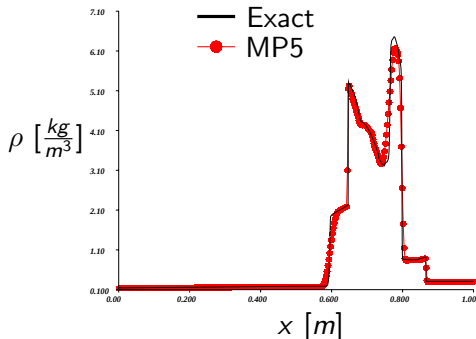
$$\hat{E} = \rho \int c_v(T) dT + \frac{1}{2} \rho u^2 \quad (3)$$

Numerical Schemes

- Monotonicity Preserving(MP) Schemes (Suresh & Huynh, 1997)
 - ▶ 5th order spatial discretization was used in conjunction with 3rd order TVD-Runge-Kutta time integration
 - ▶ Contact Discontinuities well resolved **without** the use of artificial compression methods
- Advection-Diffusion-Reaction Weighted Essential Non-Oscillatory(ADERWENO) Scheme (Titarev & Toro, 2001)
 - ▶ 5th order spatial and 3rd order temporal **without** Runge-Kutta time integration
 - ▶ Utilizes Lax-Wendroff procedure and Taylor series expansion of WENO fluxes for high order in time

Validation Studies

- Euler equation solutions using MP schemes validated for standard problems:
 - ▶ Sod's 1D Shock tube problem
 - ▶ Lax's 1D problem, shock tube with velocity field
 - ▶ Shu-Osher 1D problem, entropy wave-shock interaction
 - ▶ 1D Blastwave problem, e.g.,



300 grid points

Ideal MHD Conservation Equations

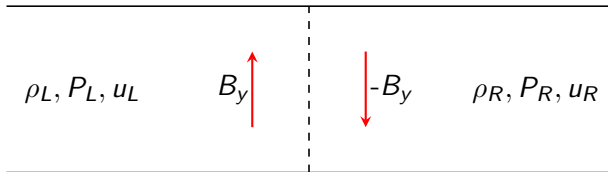
$$\mathbf{Q}_t + \mathbf{F}_x = 0$$

$$\mathbf{Q} = \begin{pmatrix} \rho_s \\ \rho \mathbf{u} \\ \mathbf{B} \\ E \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho_s u_n \\ \rho \mathbf{u} u_n + P^* \mathbf{n} - \mathbf{B} B_n \\ u_n \mathbf{B} - \mathbf{u} B_n \\ (E + P^*) u_n - B_n (\mathbf{u} \cdot \mathbf{B}) \end{pmatrix}$$

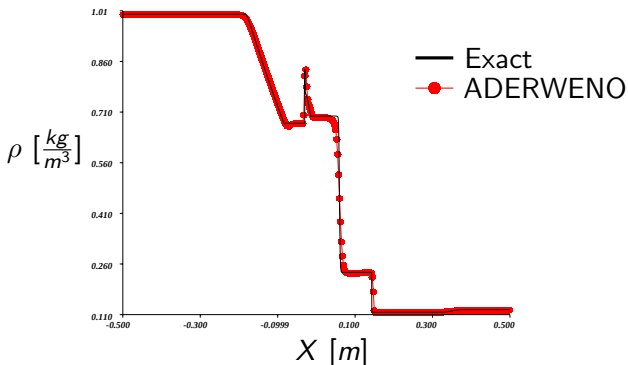
where

$$B_n = B_x n_x + B_y n_y + B_z n_z, \quad P^* = P + \frac{1}{2} \|\mathbf{B}\|^2$$

Validated for standard 1D Brio-Wu Problem, analogous to Sod's shock tube:



1D Brio-Wu validation with ADERWENO



Initial Conditions:

$$\begin{aligned} \{\rho_L, P_L, u_L, B_x, B_y\} &= \left\{1 \frac{\text{kg}}{\text{m}^3}, 10^5 \text{ Pa}, 0 \frac{\text{m}}{\text{s}}, 0.75, 1\right\} \\ \{\rho_R, P_R, u_R, B_x, B_y\} &= \left\{0.125 \frac{\text{kg}}{\text{m}^3}, 10^4 \text{ Pa}, 0 \frac{\text{m}}{\text{s}}, 0.75, -1\right\} \end{aligned}$$

Chemical Kinetics Conservation Equations

Operator-Splitting

$$\frac{d\mathbf{Q}}{dt} = \mathbf{S}$$

where

$$\mathbf{Q} = \begin{pmatrix} \rho_s \\ \rho \mathbf{u} \\ E \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} \dot{\omega}_s \\ 0 \\ \sum \dot{\omega}_s e_{0s} \end{pmatrix}$$

$$\dot{\omega}_s = \sum_r \nu_{rs} k_{fr} \prod_j [X_j]^{\nu'_{rj}} - \sum_r \nu_{rs} k_{br} \prod_j [X_j]^{\nu''_{rj}}$$

$$\nu_{rk} = \nu''_{rk} - \nu'_{rk}$$

ν''_{rk} : coefficient of k^{th} species in the r^{th} forward reaction

ν'_{rk} : coefficient of k^{th} species in the r^{th} reverse reaction

$[X_s]$: Concentration of s^{th} species

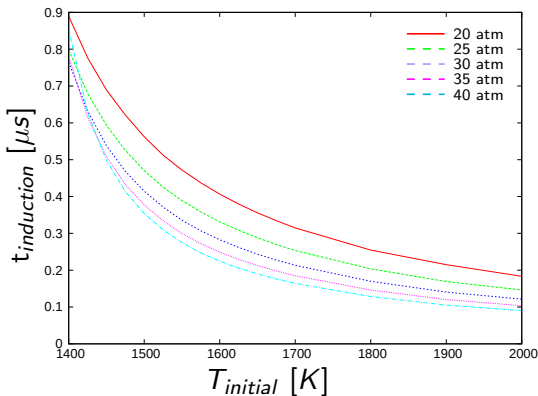
e_{0s} : Internal Energy of formation at $0K$

Kinetics of Hydrogen-Air Mixture:

- The chemistry includes eight reacting species, H_2 , O_2 , H , O , OH , HO_2 , H_2O_2 , H_2O , and the non-reacting diluent N_2 .
- Thirty eight elementary reactions are used in this mechanism and the backward rates are computed from equilibrium constants.
- Convection and Kinetics were operator split
 - ▶ Point Implicit Euler was used to solve for the kinetics

Induction Delay Time

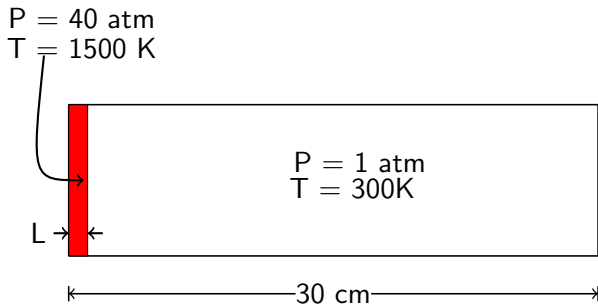
Reduced $H_2 - O_2 - N_2$ Reaction Kinetics (9 species, 38 reactions)



Can be fitted
as $t \sim \alpha(P)e^{\frac{\beta(P)}{T}}$

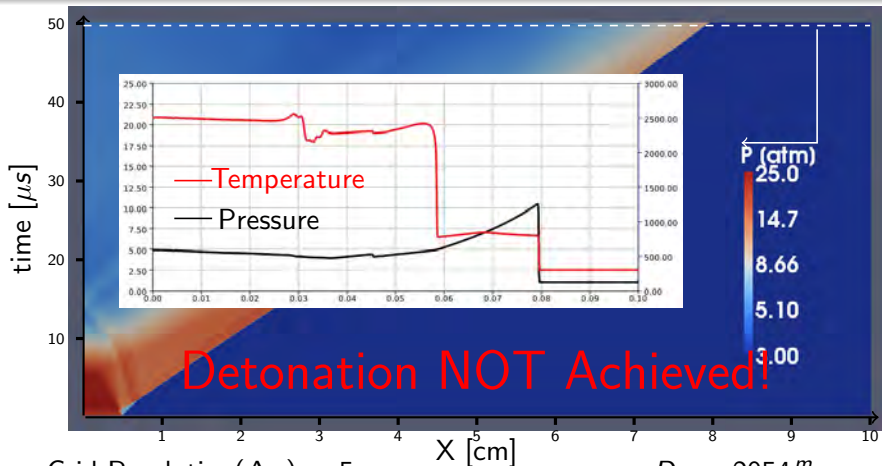
Criterion for Induction: Maximum atomic Hydrogen concentration
Mixture: Stoichiometric $H_2 - O_2 - N_2$

Detonation Test Setup



- Premixed Stoichiometric Mixture of H_2 –Air
- Closed Ends
- Spark ignited ($L = 0.25 \text{ cm}$ in the Present Study)
- $D_{cj} \approx 2054 \text{ m/s}$

Spark Ignited Detonation – Pressure Contour (MP5)

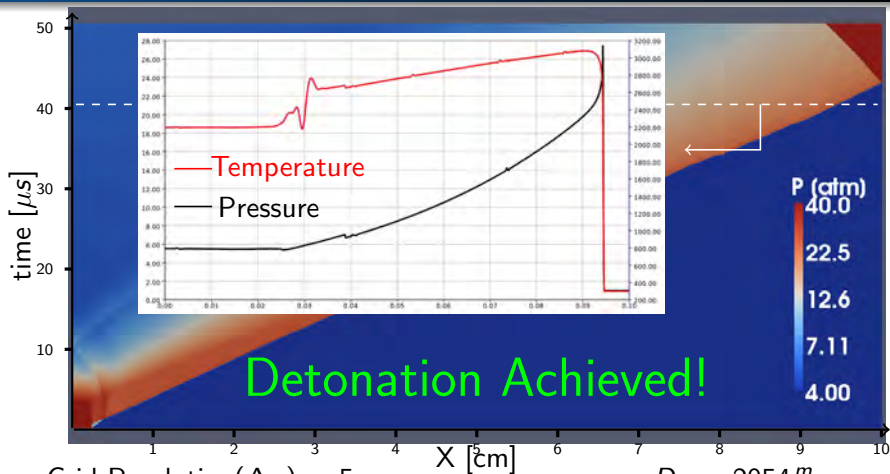


Grid Resolution(Δx) = $5\mu m$

L = 0.5 cm

$$D_{cj} = 2054 \frac{m}{s}$$

$$D = 1500 \frac{m}{s}$$

Spark Alteration ($P_{spark} = 50 \text{ atm}$, $L = .25\text{cm}$), MP5Grid Resolution(Δx) = $5\mu\text{m}$ $L = 0.25 \text{ cm}$

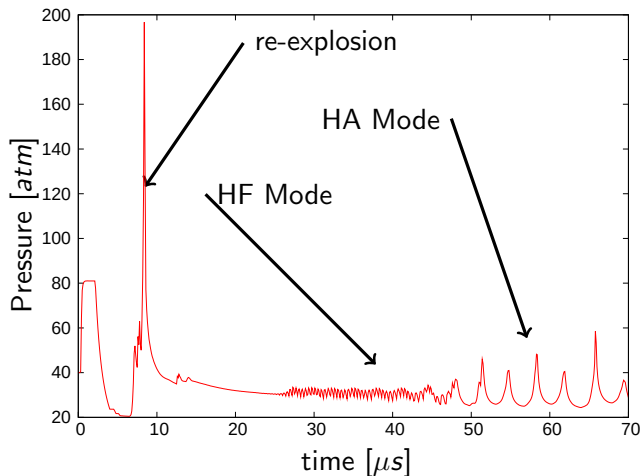
$$D_{cj} = 2054 \frac{\text{m}}{\text{s}}$$

$$D = 2031 \frac{\text{m}}{\text{s}}$$

Typical Peak Pressure vs Time Plot

Grid Resolution: $\Delta x = 2.5\mu m$

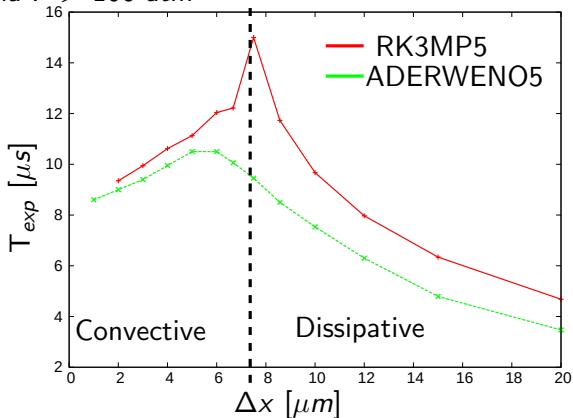
HF- High Frequency, HA- High Amplitude



Time to Re-Explosion

Time of re-explosion (T_{exp}):

- criteria $P > 100 \text{ atm}$

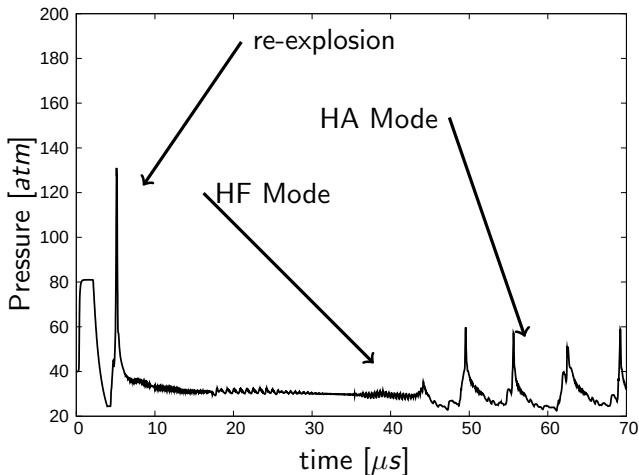


Grid Convergence

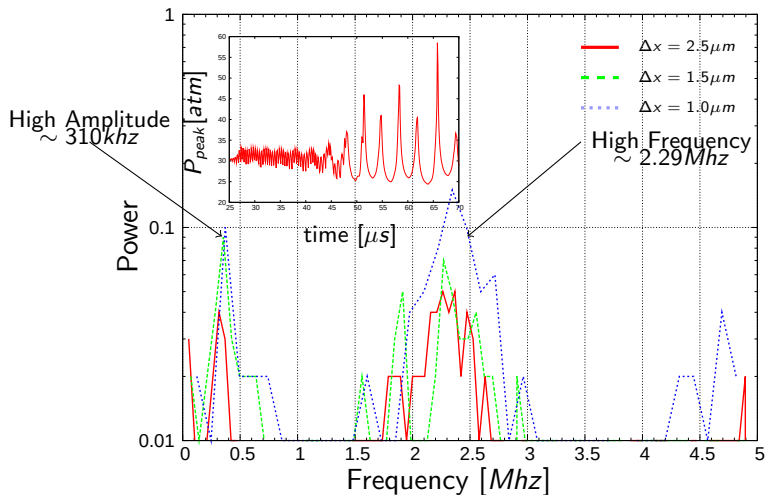
- Peak Pressure vs Time data relates macroscopic phenomena to microscopic phenomena
- Spectral content of the High Frequency and High Amplitude Modes for various grid resolution can be used to determine convergence
- High Frequency modes were inconsistent as the grid resolution increased to $\Delta x \geq 7.5\mu m$

Typical Peak Pressure vs Time Plot

Grid Resolution: $\Delta x = 12.5\mu m$

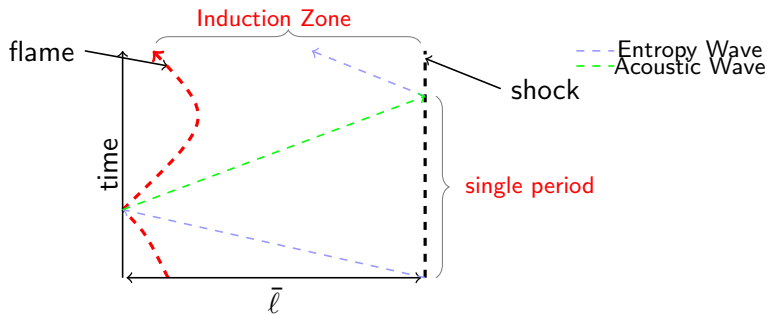


Spectral Convergence



Simplified Model

Induction Zone Dynamics

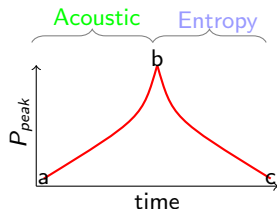


$$\left. \frac{dx}{dt} \right|_{\text{entropy}} = u_2(x, t) \quad (4)$$

$$\left. \frac{dx}{dt} \right|_{\text{acoustic}} = c(x, t) - u_2(x, t) \quad (5)$$

where $u_2(x, t) = |u(x, t) - D(t)|$ (detonation ref. frame)

Verify Simple Model



$$T = \frac{\bar{\ell}}{c_a + u_a - \bar{D}_{a \rightarrow b}} + \frac{\ell}{u_b - \bar{D}_{b \rightarrow c}} \quad (6)$$

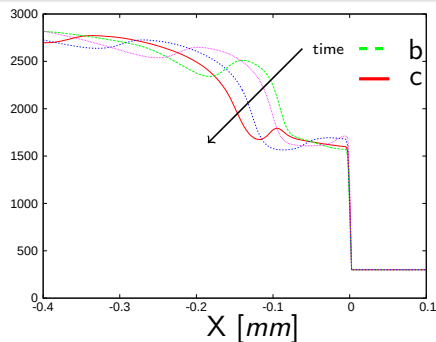
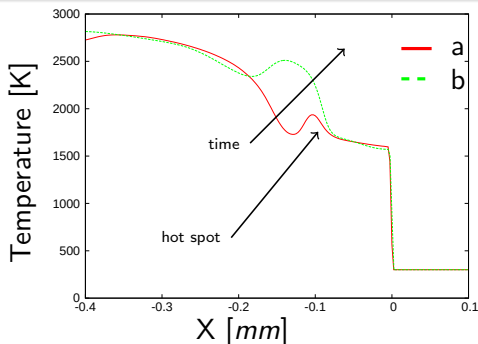
$$f = T^{-1}, \text{ frequency}$$

Assumptions for zeroth order approximation:

- $\bar{D} = \frac{1}{T} \int D(t) dt$
- $\gamma \approx 1.28$
- $T, P, \rho, u \rightarrow F(x, t), \quad \frac{\partial F(x, t)}{\partial t} \simeq 0 \ \& \ \frac{\partial F(x, t)}{\partial x} \simeq 0$

Verify Simple Model

High Frequency Mode

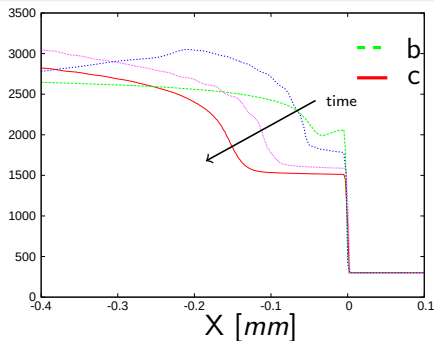
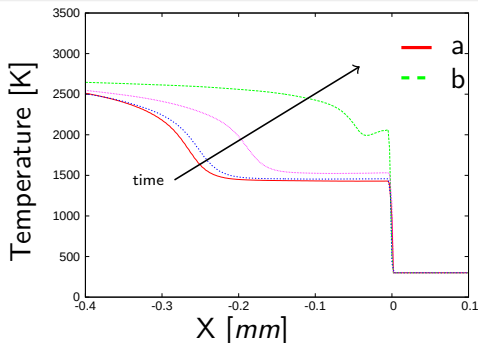


a: $29.1\mu s$ b: $29.3\mu s$ c: $29.5\mu s$

$f \approx 2.08 \text{ Mhz}$, In good agreement with spectral analysis
 $(2.29 \pm 0.4 \text{ Mhz})$

Verify Simple Model

High Amplitude Mode



a: $56.7\mu s$ b: $58.3\mu s$ c: $60.1\mu s$

$f \approx 310 \text{ kHz}$, In great agreement with spectral analysis
 $(310 \pm 40 \text{ kHz})$

Conclusions

- Same fundamental dynamics for High Frequency and High Amplitude Modes
- The location of the hot spot, whether within the flame or reaction zone, plays a key role in pressure oscillations.
 - ▶ 'hot spot' inhibits progress of flame toward shock by pre-igniting fluid, thus suppressing the peak amplitude of pressure
- HF Mode: "hotspot" well resolved within induction zone, leading to small fluctuations in Pressure
- HA Mode: fluctuations are within flame, allowing for more energy release (via Swacer effect)

Future Work

- Conduct similar test with a seeded species of low ionization energy and direct initiation (Hydrocarbon fuel)
 - ▶ Observe how ionization processes effect the induction region and large scale phenomena
- Apply B-field of varying strength

Backup

MHD Effects

Additional Physics added in MHD

$$\begin{aligned}\vec{F} &= \vec{J} \times \vec{B} && \text{Lorentz Force} \\ Q &= \vec{J} \cdot \vec{E} && \text{Joule Heating}\end{aligned}\tag{7}$$

Questions:

- How will energy extraction/introduction via joule heating effect the stability of the detonation?
- How will the magnetic Pressure evolution effect the Reaction Zone & detonation stability?