Linear stability and receptivity of planar idealized one-reaction detonation to three-dimensional perturbations

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[1] By Chiquete, C., Shalaev, I. and Tumin, A., January 2008

Detonation waves

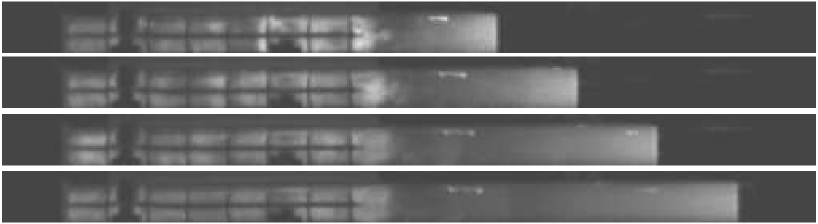
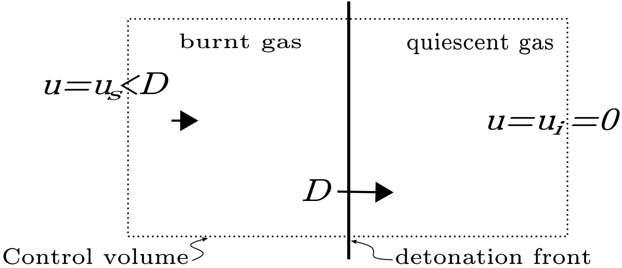


Figure: High speed camera snapshots of detonation wave propagation in a tube. Constant velocity of detonation front is shown. (General Electric Global Research, 2006)

- Detonations waves are supersonic combustion-driven shock waves with applications in Pulse Detonation Engine (PDE), and supernova models.

Detonation waves - The simplest theory



- Detonation waves can be idealized as a one-dimensional traveling discontinuity in pressure, temperature etc...
- Simplest theory is named after Chapman (1899) and Jouguet (1906) which assumes that reaction takes place entirely on the planar shock wave front and reaction products are in thermodynamic equilibrium.

Conservation relations centered on shock

- Attaching our coordinate system to the shock results in the following conservation relations:
  - Conservation of mass:

$$\rho_s(D-u_s)=\rho_i D$$

  - Conservation of momentum:

$$p_s-p_i=\rho_s u_s D$$

  - Conservation of energy:

$$E_s+p_s/\rho_s+\frac{1}{2}(D-u_s)^2=E_i+p_i/\rho_i+\frac{1}{2}D^2$$

  - *i*-initial state in front of shock, *s*-state just after shock.

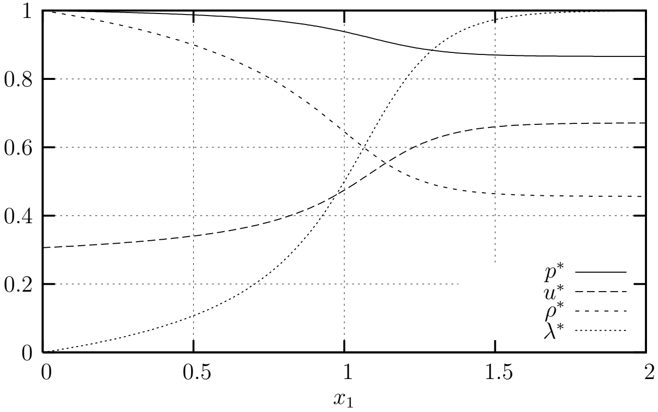
ZND theory

- Extended theory called ZND theory after **Z**el'dovich (1940), von **N**eumann (1942), **D**oering (1943).
- In this case, the Arrhenius reaction rate is used:

  $$r = \frac{D\lambda}{Dt} = k(1-\lambda)\exp(-\tilde{E}/R_g T)$$

  Reaction progress variable transitions from $\lambda = 0$ (no reaction) to $\lambda = 1$ (completion of reaction).
- It leads to a finite length reaction zone and $E(p, v, \lambda) = pv/(\gamma - 1) - \lambda q$ where $\lambda \in [0, 1]$.

Steady state plots



- Flow is steady with coordinates attached to shock front.
- Distance from shock x_1 is dimensionless and is scaled with half reaction zone length.

The governing equations in sho ck frame

- Governing equations are reactive Euler equations.
- The transformations $x_1 = x_1^l - Dt - \psi(x_2, x_3, t)$ and $u_1 = u_1^l - D$ lead to:

$$\begin{aligned}
&\frac{Dv}{Dt} - v\nabla\cdot\mathbf{u} + v\nabla\psi\cdot\frac{\partial\mathbf{u}}{\partial x_1} - \frac{D\psi}{Dt}\frac{\partial v}{\partial x_1} = 0\\
&\frac{D\mathbf{u}}{Dt} + v\nabla p - \frac{\partial\mathbf{u}}{\partial x_1}\frac{D\psi}{Dt} - v\frac{\partial p}{\partial x_1}\nabla\psi = 0\\
&\frac{Dp}{Dt} + p\frac{Dv}{Dt} - \frac{D\psi}{Dt}\frac{\partial p}{\partial x_1} - \gamma p\left(\frac{\partial\mathbf{u}}{\partial x_1}\cdot\nabla\psi\right) = \frac{(\gamma-1)Qr}{v}\\
&\frac{D\lambda}{Dt} - \frac{D\psi}{Dt}\frac{\partial\lambda}{\partial x_1} = r
\end{aligned}$$

- Velocity vector $\mathbf{u} = (u_1, u_2, u_3)^T$, Material derivative $D/Dt = \partial/\partial t + \mathbf{u}\cdot\nabla$, ψ perturbation to shock front position.

Matrix form of equations

- Define $\mathbf{z} = (v, u_1, u_2, u_3, p, \lambda)^T$.
- Introduce superposition: $\mathbf{z} = \mathbf{z}^*(x_1) + \mathbf{z}'(x_1, x_2, x_3, t)$,

$$\boxed{\frac{\partial \mathbf{z}'}{\partial t} + \mathbf{A}_1 \frac{\partial \mathbf{z}'}{\partial x_1} + \mathbf{A}_2 \frac{\partial \mathbf{z}'}{\partial x_2} + \mathbf{A}_3 \frac{\partial \mathbf{z}'}{\partial x_3} + \mathbf{C}\mathbf{z}' - \mathbf{g}_t \frac{\partial \psi}{\partial t} - \mathbf{g}_2 \frac{\partial \psi}{\partial x_2} - \mathbf{g}_3 \frac{\partial \psi}{\partial x_3} = 0}$$

- Matrices $\mathbf{A_1}, \mathbf{A_2}, \mathbf{A_3}$ and $\mathbf{C}$ are 6×6 and depend on x_1, and finally $\mathbf{g}_t, \mathbf{g}_2$ and $\mathbf{g}_3$ are column vectors of size 6×1 and depend on x_1 as well.
- We permit perturbations incoming from the gas in front of the shock, and obtain the following BC:

$$\boxed{\mathbf{z}'\left(0_+, t\right) = \mathbf{Y}\mathbf{z}'\left(0_-, t\right) + \mathbf{h}_t \frac{\partial \psi}{\partial t} + \mathbf{h}_2 \frac{\partial \psi}{\partial x_2} + \mathbf{h}_3 \frac{\partial \psi}{\partial x_3}}$$

where $\mathbf{h}_t$, $\mathbf{h}_2$, and $\mathbf{h}_3$ are 6×1 and $\mathbf{z}'(0_-, t)$ is considered known.

The initial value problem (IVP)

- We define the IVP by setting

$$t = 0: \ \mathbf{z}'(x_1, x_2, x_3, 0) = \mathbf{z}_0(x_1, x_2, x_3), \ \psi(x_2, x_3, 0) = 0$$

- Therefore we have PDE system of linear equations with coefficient matrices which depend on x_1 through the base flow $\mathbf{z}^* = (v^*, u^*, 0, 0, p^*, \lambda^*)$.
- To solve we use Fourier transform in x_2 and x_3 and take Laplace transform in time $t \in (0, \infty)$.

$$\bar{\mathbf{z}}(x_1, \alpha, \beta, \tau) = \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty e^{-i(\alpha x_2 + \beta x_3) - \tau t} \mathbf{z}'(x_1, x_2, x_3, t)\, dx_2 dx_3 dt$$

Inhomogeneous linear ODE system with non-constant coefficients

- We also transform the BC on the shock (i.e. $x_1 = 0$),

$$\bar{\mathbf{z}}\left(0_{+}\right) = \mathbf{Y}\bar{\mathbf{z}}\left(0_{-}\right) + \left(\tau\mathbf{h}_t + i\alpha\mathbf{h}_2 + i\beta\mathbf{h}_3\right)\bar{\psi}$$

- We want bounded solutions as $x_1 \to \infty$.
- The full equations are therefore:

$$\mathbf{A}_1\frac{d\bar{\mathbf{z}}}{dx_1} + \left(i\alpha\mathbf{A}_2 + i\beta\mathbf{A}_3 + \mathbf{C} + \tau\mathbf{I}\right)\bar{\mathbf{z}} = \left(\tau\mathbf{g}_t + i\alpha\mathbf{g}_2 + i\beta\mathbf{g}_3\right)\bar{\psi} + \hat{\mathbf{z}}_0\left(x_1\right)$$

- Can rewrite problem as the following:

$$\frac{d\bar{\mathbf{z}}}{dx_1} + \mathbf{P}\bar{\mathbf{z}} = \mathbf{F}$$

$$\mathbf{P} = \mathbf{A}_1^{-1}[i\alpha\mathbf{A}_2 + i\beta\mathbf{A}_3 + \mathbf{B} + \tau\mathbf{I}]$$

$$\mathbf{F} = \mathbf{F}_1 + \mathbf{F}_2\bar{\psi}$$

$$\mathbf{F}_1 = \mathbf{A}_1^{-1}\hat{\mathbf{z}}_0, \mathbf{F}_2 = \mathbf{A}_1^{-1}\left(\tau\mathbf{g}_t + i\alpha\mathbf{g}_2 + i\beta\mathbf{g}_3\right)$$

- For linear problem: Get fundamental solutions of homogeneous problem, then get particular solution.

Asymptotics and solution

- Full problem will have to be solved numerically.
- However, we can analyze problem solution analytically for $x_1 \longrightarrow \infty$ or as the coefficient matrices tend to constants.
- For example we know that $\mathbf{P} \rightarrow \mathbf{P}_\infty$ exponentially in x_1 outside the reaction zone.
- The system of 6 ODE's will have 6 homogeneous solutions of the form $\mathbf{z}_j = \mathbf{z}_{j\infty} \exp(\mu_j x)$.

Fundamental solutions

- It turns out that $\mathrm{Re}(\mu_1) > 0$ and $\mathrm{Re}(\mu_j) < 0$, for $j > 1$.

$$\mu_1 = \frac{u_\infty^* \tau + \sqrt{\tau^2 + k^2(c_\infty^2(1 - M_\infty^2))}}{c_\infty^2(1 - M_\infty^2)}, \; k^2 = \alpha^2 + \beta^2.$$

- Get bounded solution through *variation of parameters method*:

$$\bar{\mathbf{z}} = \sum_{j=2}^{6} \left(a_j + \int_0^{x_1} \mathbf{y}_j \cdot \mathbf{F} dx_1 \right) \bar{\mathbf{z}}_j + \bar{\mathbf{z}}_1 \int_\infty^{x_1} \mathbf{y}_1 \cdot \mathbf{F} dx_1$$

- Inverse Laplace transform in t:

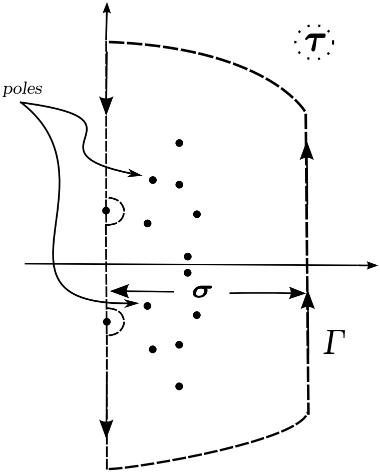
$$\hat{\mathbf{z}}(x_1, t, \alpha, \beta) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} \bar{\mathbf{z}}(x_1, \tau; \alpha, \beta) e^{\tau t} d\tau$$

- Can also get displacement of the shock perturbation $\bar{\psi}$,

$$\bar{\psi} = -\frac{\mathbf{y}_1\left(0\right) \cdot \mathbf{Y}\bar{\mathbf{z}}\left(0_-\right) + \int_0^\infty \left(\mathbf{y}_1 \cdot \mathbf{F}_1\right) dx_1}{V(\tau, \alpha, \beta)}$$

- $\bar{\psi}$ appears as a factor in our solution for $\bar{\mathbf{z}}$.
- If $V(\tau, \alpha, \beta) = 0$ then we have singularity in the complex plane of τ for $\bar{\mathbf{z}}$ $\Rightarrow$ residue value!

Inverse Laplace transform in time



- The Bromwich integral must be defined from $\sigma - i\infty$ to $\sigma + i\infty$ where $\sigma > 0$ is chosen to close the path to the right of any singularities.
- It turns out that having $\mathrm{Re}(\tau) > 0$ is crucial for causality.
- We close path with arcs of infinite radii.

- Therefore we have contribution from discrete and continuous spectrum.

$$\hat{\mathbf{z}}\left(x_1,\alpha,\beta,t\right)=\sum_j R_j\hat{\mathbf{z}}_{dmj}\left(x_1,\alpha,\beta\right)e^{\tau_j t}+\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\bar{\mathbf{z}}\left(x_1,\alpha,\beta,\tau\right)e^{\tau t}d\tau$$

- We can get quite simply the amplitudes of the unstable modes:

$$R_j=-\frac{\left[\mathbf{y}_1\left(0\right)\cdot\mathbf{Y}\bar{\mathbf{z}}\left(0_-\right)+\int_0^\infty\left(\mathbf{y}_1\cdot\mathbf{F}_1\right)dx_1\right]_{\tau=\tau_j}}{\left(\partial V/\partial\tau\right)_{\tau=\tau_j}}$$

- Unstable modes determined when $V(\tau_j,\alpha,\beta)=0$.

Eigenvalues for $\alpha = 0, \beta = 0$.

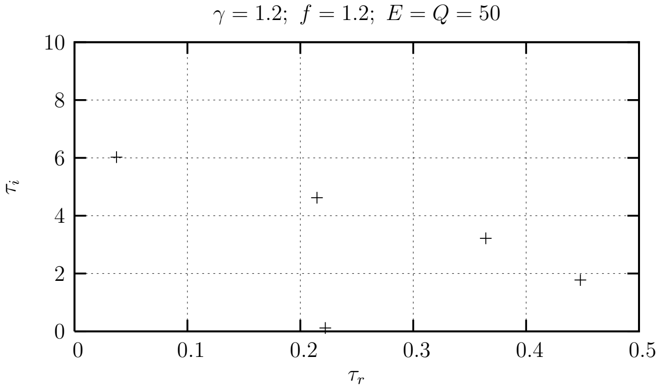


Figure: Eigenvalue map for one-dimensional perturbations obtained with the help of three-domain spectral collocation method. γ is specific heats ration, $f = (D/D_{CJ})^2$ is overdrive factor, E is dimensionless activation energy, and Q is dimensionless heat release

Eigenvalues evolution as α and β are varied.

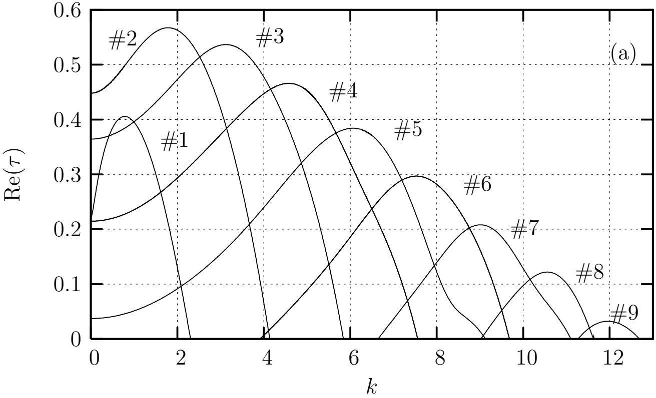


Figure: Real part of eigenvalues with increasing α and β. Here: $k = \sqrt{\alpha^2 + \beta^2}$

Examples of receptivity analysis

- Can introduce perturbations into the gas behind the front of the detonation front or in the quiescent zone ahead.
  - For example we could make the introduce an initial perturbation of the form

    $$\mathbf{z}_0(x_1, x_2, x_3) = \mathbf{z}_{rc1}\delta(x_1 - x_{10})\delta(x_2)\delta(x_3),$$
    $$\mathbf{z}_{rc} = (1, 0, 0, 0, -\gamma p^*(x_{10})/v^*(x_{10}), 0)^T$$

    and vary the location of the localized *spike*, in x_1.
  - A spatial perturbation in the density ahead therefore gets transformed into a temporal one at in the front attached coordinates:

    $$\mathbf{z}(0_-) = \mathbf{z}_q \sin \omega t$$
    $$\mathbf{z}_q = (1, 0, 0, 0, 0, 0)^T$$

Reaction zone perturbations

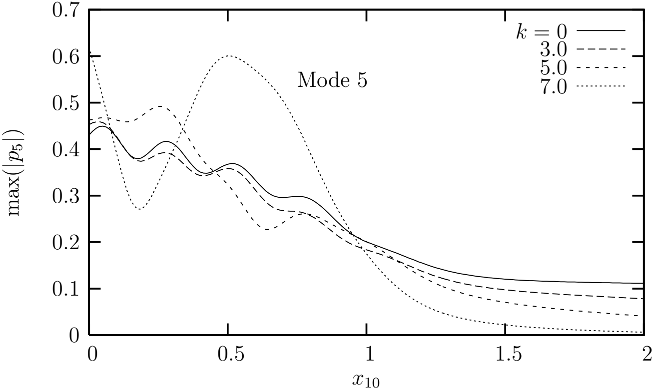


Figure: Maximum of the pressure perturbation in the discrete mode 5 when the initial perturbation is located at x_{10}. Adiabatic perturbation.

Conclusion and summary

- The IVP approach to the stability of detonations was developed.
- Consideration of asymptotics leads to full solution of the IVP problem.
- Solution is represented as inputs from discrete spectrum (poles in complex plane of τ) and also from continuous spectrum.
- Results show detonation wave is more receptive to 3D perturbations than 1D ones.
- Examples of receptivity analysis is shown.