Detonation wave problems: modeling, numerical simulations and linear stability

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Main Goals:

- Influence of the reaction heat on the steady detonation behavior;
- Linear stability spectrum of the steady detonation;
- Emphasis on the influence of the reaction heat and of the activation energy.

Structure

- Outline;
- Reactive Boltzmann Equation and its properties;
- Hydrodynamic Limit;
- Steady detonation wave;
- Steady detonation wave - Numerical results;
- Linear stability - Modeling;
- Linear stability - Numerical procedure;
- Linear stability - Numerical results.

Outline

The gas has two constituent, A and B, with the same mass m and binding energies E_A and E_B, respectively. The constituent molecules collide among themselves through elastic scattering and undergo a reversible chemical reaction of type

$$A + A \rightleftharpoons B + B.$$

External forces and internal degrees of freedom are neglected. The collisions obey the classical laws of mechanics (non-relativistic and non quantum effects)

Reactive Boltzman Equation

$$f_\alpha \equiv f(x, \mathbf{c}_\alpha, t) \qquad \alpha = A, B. \tag{1}$$

$$\frac{\partial f_\alpha}{\partial t} + \sum_{i=1}^{3} c_i^\alpha \frac{\partial f_\alpha}{\partial x_i} = \sum_{\beta=A}^{B} \mathcal{Q}_{\alpha\beta}^E + \mathcal{Q}_\alpha^R. \tag{2}$$

Elastic collision terms are defined by

$$\mathcal{Q}_{\alpha\beta}^E = \int \left(f'_\alpha f'_\beta - f_\alpha f_\beta\right) d^2 \left(g_{\beta\alpha} \cdot \mathbf{k}_{\beta\alpha}\right) d\mathbf{k}_{\beta\alpha} d\mathbf{c}_\beta, \tag{3}$$

and reactive collision terms by

$$\mathcal{Q}_A^R = \int \left[f_B f_{B1} - f_A f_{A1}\right] \sigma_A^\star \left(g_A \cdot \mathbf{k}_A\right) d\mathbf{k}_A d\mathbf{c}_{A1}, \tag{4}$$

$$\mathcal{Q}_B^R = \int \left[f_A f_{A1} - f_B f_{B1}\right] \sigma_B^\star \left(g_B \cdot \mathbf{k}_B\right) d\mathbf{k}_B d\mathbf{c}_{B1}. \tag{5}$$

Reactive Boltzman Equation

Reactive step cross sections with activation energy

$$\sigma_\alpha^\star = \begin{cases} 0 & \textit{for} \quad \gamma_\alpha < \varepsilon_\alpha^\star \\ d_r^2 & \textit{for} \quad \gamma_\alpha > \varepsilon_\alpha^\star \end{cases} \tag{6}$$

$$\gamma_\alpha = \frac{m g_\alpha^2}{4kT}, \quad \varepsilon_A^\star \equiv \varepsilon^\star = \frac{\varepsilon}{kT}, \quad \varepsilon_B^\star \equiv \varepsilon^\star - Q_R^\star, \quad Q_R^\star \equiv \frac{Q_R}{kT}, \tag{7}$$

where Q_R is the reaction heat defined by

$$Q_R = 2\,(E_B - E_A) \tag{8}$$

Reactive Boltzman Equation

Some properties:

Proposition

The elastic collision terms are such that

$$\int_{\mathbb{R}^3} \mathcal{Q}_\alpha^E d\mathbf{c}_\alpha = 0 \qquad \alpha = A, B. \tag{9}$$

Proposition

The reactive terms satisfy the following property:

$$\int_{\mathbb{R}^3} \mathcal{Q}_A^R d\mathbf{c}_A = -\int_{\mathbb{R}^3} \mathcal{Q}_B^R d\mathbf{c}_B. \tag{10}$$

Reactive Boltzman Equation

Definition

A function ψ_α *is a* **collision invariant** *in the velocity space if*

$$\sum_{\alpha=A}^{B} \int_{\mathbb{R}^3} \psi_\alpha \left(\mathcal{Q}_\alpha^E + \mathcal{Q}_\alpha^R \right) d\mathbf{c}_\alpha = 0 \tag{11}$$

Proposition

The functions ψ_α *defined by* $\psi_\alpha = 1$, $\psi_\alpha = m_\alpha c_i^\alpha$, $i = 1, 2, 3$ *and* $\psi_\alpha = E_\alpha + \frac{1}{2}\mathbf{c}_\alpha^2 m_\alpha$ *are collision invariants.*

These are related to the conservation of number density, linear momentum components and total energy of the mixture.

Reactive Boltzman Equation

Proposition

If all constituents are at the same temperature, the elastic equilibrium distribution function is a Maxwellian:

$$f_\alpha^M = n_\alpha \left(\frac{m_\alpha}{2\pi kT}\right)^{\frac{3}{2}} Exp\left[-\frac{m_\alpha \xi_\alpha^2}{2kT}\right]. \tag{12}$$

Proposition

The thermodynamical (elastic and chemical) equilibrium is characterized by Maxwellians constrained to the mass action law

$$\frac{Q_R}{kT} = \ln\left(\frac{n_A^{\mathrm{eq}}}{n_B^{\mathrm{eq}}}\right)^2. \tag{13}$$

Reactive Boltzman Equation

Proposition

If we consider the distribution function f_α uniform in space for every $\alpha = A, B$, the functional $\mathcal{H}$ defined by

$$\mathcal{H}(t) = \sum_{\alpha=A}^{B} \int_{\mathbb{R}^3} f_\alpha \log(f_\alpha)\, d\mathbf{c}_\alpha \tag{14}$$

respects the following conditions:

a) $\frac{d}{dt}\mathcal{H}(t) \leq 0$

b) $\frac{d}{dt}\mathcal{H}(t) = 0$ *if and only if the gas is in thermodynamical equilibrium.*

Hydrodynamic limit

Balance equation for the number density of constituent A and Conservation equations for the number density, linear momentum components and total energy of the mixture

1. Multiply the Boltzmann equation by $\psi_\alpha = \delta_{A\alpha}$, $\psi_\alpha = 1$, $\psi_\alpha = m_\alpha c_i^\alpha$, $i = 1, 2, 3$ and $\psi_\alpha = E_\alpha + \frac{1}{2}\mathbf{c}_\alpha^2 m_\alpha$
2. Integrate over $\mathbf{c}_\alpha$
3. Sum over all constituents

This equation system is not closed. To close the system one passes to the hydrodynamic limit, which requires a solution of the Boltzmann equation.

Hydrodynamic limit

In a chemical regime in which elastic collisions are more frequent than reactive encounters, the solution of the BE is (see [KS07])

$$f_\alpha^{(0)} = f_\alpha^M \left[1 + \omega \left(\frac{15}{8} - \frac{5m(c_\alpha - v)^2}{4kT} + \frac{m^2(c_\alpha - v)^4}{8k^2T^2}\right)\right], \quad (15)$$

where

$$\begin{aligned}\omega &= x_A^2 \left(\frac{d}{d_r}\right)^2 \frac{Q_R^\star}{8} \Big[\left(1 + 2Q_R^\star - 3Q_R^\star\varepsilon_A^\star - Q_R^{\star 2} + \varepsilon_A^\star - 2\varepsilon_A^{\star 2}\right) e^{-\mathcal{A}^\star} \\ &\quad - \left(1 - Q_R^\star - Q_R^\star\varepsilon_A^\star + \varepsilon^\star - 2\varepsilon_A^{\star 2}\right)\Big] e^{-\varepsilon_A^\star}. \quad (16)\end{aligned}$$

Hydrodynamic limit

The hydrodynamic governing equations are

$$\frac{\partial}{\partial t} n_A + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(n_A v_i) = \tau_A, \tag{17}$$

$$\frac{\partial}{\partial t} n + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(n v_i) = 0 \tag{18}$$

$$\sum_{i=1}^{3} \frac{\partial}{\partial t}(\varrho v_i) + \sum_{i=1}^{3}\sum_{j=1}^{3} \frac{\partial}{\partial x_j}(p\delta_{ij} + \varrho v_i v_j) = 0 \tag{19}$$

$$\frac{\partial}{\partial t}\left[\frac{3}{2} nkT + \sum_{\alpha=A}^{B} n_\alpha E_\alpha + \frac{1}{2}\varrho v^2\right] + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left[\sum_{j=1}^{3} p\delta_{ij} v_j + \left(\frac{3}{2} nkT + \sum_{\alpha=A}^{B} n_\alpha E_\alpha + \frac{1}{2}\varrho v^2\right) v_i\right] = 0. \tag{20}$$

Hydrodynamic limit

The governing equations are the Euler equations with the reaction rate τ_A constructed from a kinetic approach, with the form

$$\tau_A = -4n_A^2 d_r^2 \sqrt{\frac{\pi kT}{m}}\, e^{-\varepsilon_A^\star}\left[1+\varepsilon_A^\star + \frac{x_A^2}{128}\left(\frac{d}{d_r}\right)^2 Q_R^\star \right. \tag{21}$$

$$\left. \times \left(1+Q_R^\star + Q_R^\star\varepsilon_A^\star + \varepsilon_A^\star - 2\varepsilon_A^{\star 2}\right)\left(4\varepsilon_A^{\star 3} - 8\varepsilon_A^{\star 2} - \varepsilon_A^\star - 1\right) e^{-\varepsilon_A^\star}\right].$$

It is possible to recognize the influence of the reaction heat $Q_R^\star$ and of the activation energy $\varepsilon_A^\star$.

Steady detonation

Outline:

- One dimensional detonation wave
- Wave velocity correspondent to an overdriven detonation

Steady detonation wave

Zeldovich, von Neumann and Doering.

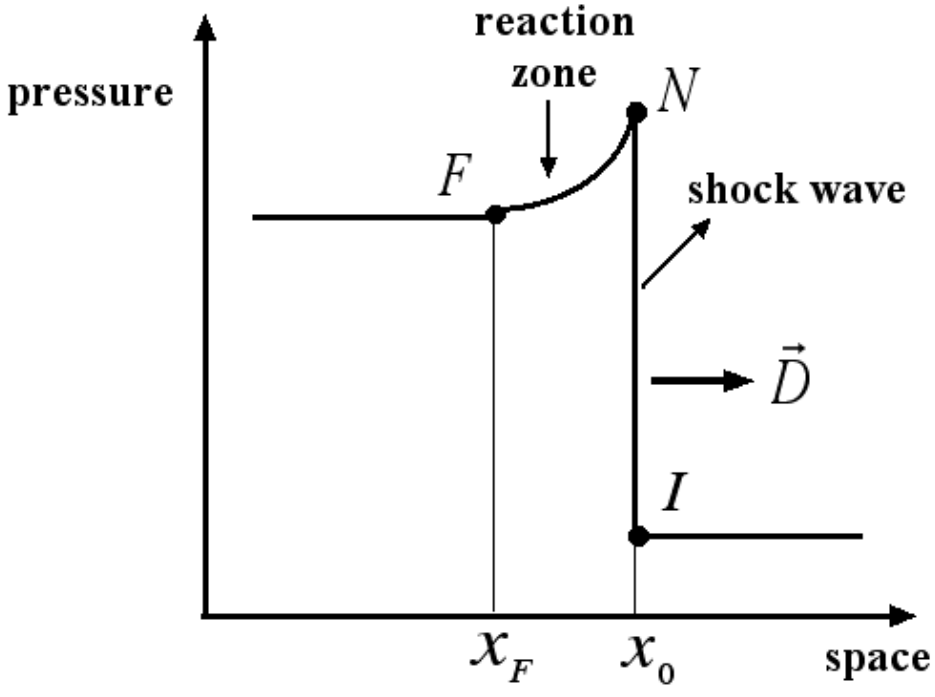


Figure: ZND configuration of a steady detonation wave profile for the mixture pressure.

Steady detonation wave

The one dimensional governing equations in the the steady frame attached to the shock have the form

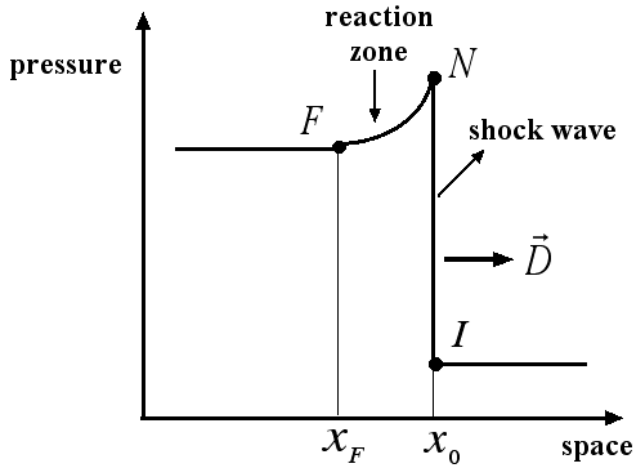
$$\frac{d}{dx}\Big[\,(v-D)\,n_A\Big] = Dt_c\tau_A, \tag{22}$$

$$\frac{d}{dx}\Big[\,(v-D)\,(n_A+n_B)\,\Big] = 0, \tag{23}$$

$$\frac{d}{dx}\Big[\,(v-D)\,\varrho v + nkT\Big] = 0, \tag{24}$$

$$\frac{d}{dx}\left[(v-D)\left(\frac{3}{2}nkT + \frac{\varrho v^2}{2} + E_A n_A + E_B n_B\right) + nkTv\right] = 0. \tag{25}$$

Steady detonation wave



- Step 1 (state N)

- No chemistry involved;
- Shock Problem (algebraic);
- Rankine-Hugoniot conditions:

$$n_A\,(v-D) = -n_A^+ D \tag{26}$$

$$n\,(v-D) = -n^+ D \tag{27}$$

$$\varrho v\,(v-D) + nkT = n^+ kT^+ \tag{28}$$

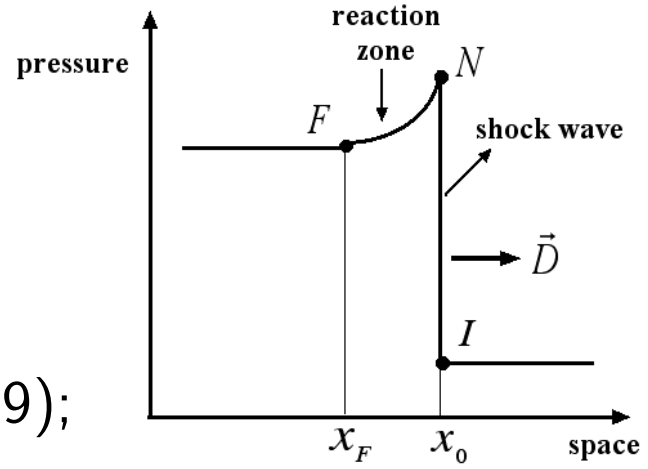
$$\left(\frac{3}{2}nkT + \frac{\varrho v^2}{2} + E_A n_A + E_B n_B\right)(v-D) + nkTv$$

$$= -\left(\frac{3}{2}n^+ kT^+ + E_A n_A^+ + E_B n_B^+\right) D. \tag{29}$$

Steady detonation wave

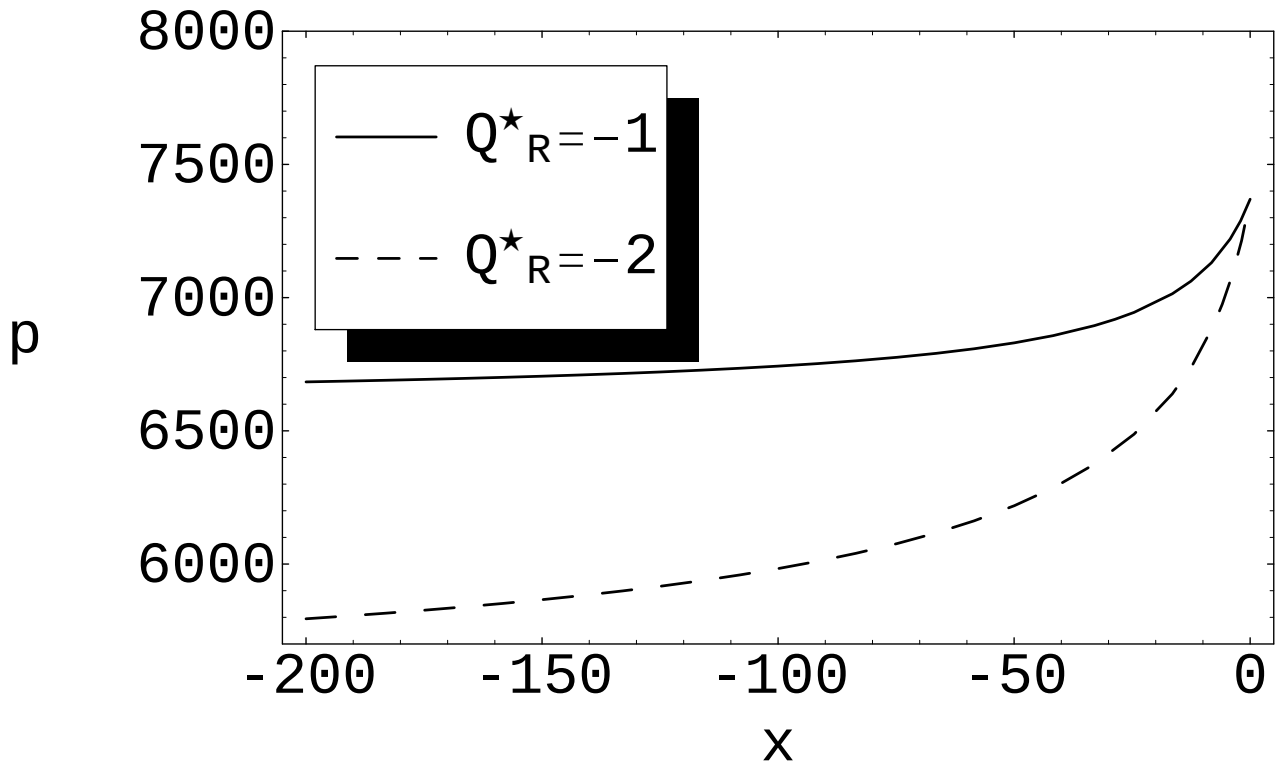
- Step 2 (states R, F)

- Relevant chemistry;
- Detonation Problem (Differential);
- Rankine-Hugoniot conditions (27–29);
- Rate law:



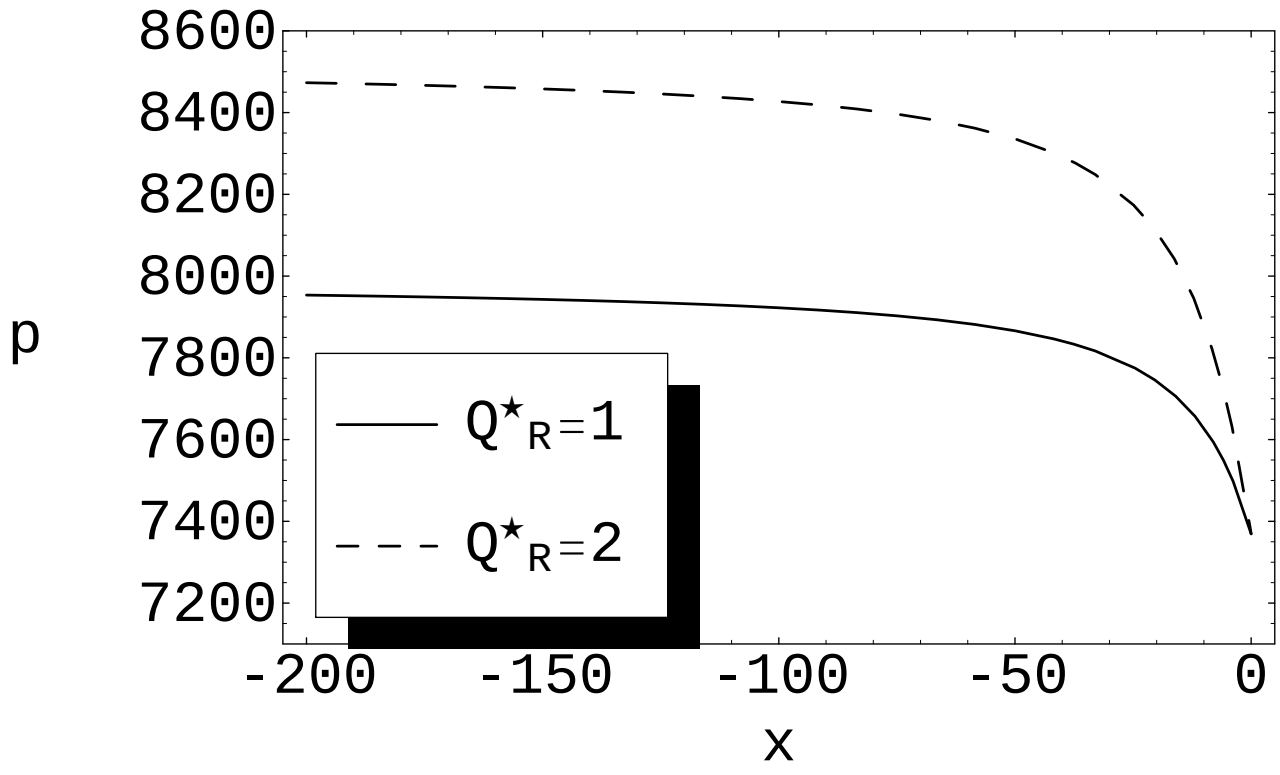
$$\frac{d}{dx} n_A = \frac{D t_c \tau_A}{v - D + n_A \frac{dv}{dn_A}} , \tag{30}$$

Steady detonation wave - Numerical results



Exothermic reaction:
$Q_R^\star = -1$ (solid line) and $Q_R^\star = -2$ (dashed line).

Steady detonation wave - Numerical results



Endothermic reaction:
$Q_R^\star = 1$ (solid line) and $Q_R^\star = 2$ (dashed line).

Linear stability - Modeling

Outline:

- One dimension linear stability;
- Small rear boundary perturbations;

Linear stability - Modeling

- Step 1 (Technical)

Transform the one-dimensional closed governing equations (22–25) to the perturbed wave coordinate x, which measures the distance from the perturbed shock, namely

$$x = x^{\ell} - \psi(t), \qquad \text{with} \qquad \psi(t) = Dt + \widetilde{\psi}(t). \tag{31}$$

The shock position is $x = 0$ and the shock velocity is $D(t) = D + \widetilde{\psi}'(t)$.

- Step 2 (Normal mode approach)

A normal mode expansion of the steady state variables,

$$z(x,t) = z^*(x) + e^{at}\,\overline{z}(x), \qquad \psi(t) = \overline{\psi}\,e^{at}, \qquad a,\,\overline{\psi} \in \mathbb{C}, \quad (32)$$

State vector: $z = [n_A\ n\ v\ p]^T$
Steady solution: $z^*(x)$
Spatial disturbances: $\overline{z}(x)$
Disturbance amplitude parameter: $\overline{\psi}$
Eigenvalue: a
Perturbation growth rate: $\mathrm{Re}\,a$
Perturbation frequency: $\mathrm{Im}a$

- Step 3 (Linearization)

Linearize the resulting governing equations:

$$Da\overline{n}_A+(v^*-D)\frac{d}{dx}\overline{n}_A+(\overline{v}-Da)\frac{d}{dx}n_A^*+\overline{n}_A\frac{d}{dx}v^*+n_A^*\frac{d}{dx}\overline{v}=\overline{\tau}_A, \quad (33)$$

$$Da\overline{n}+(v^*-D)\frac{d}{dx}\overline{n}+(\overline{v}-Da)\frac{d}{dx}n^*+\overline{n}\frac{d}{dx}v^*+n^*\frac{d}{dx}\overline{v}=0, \quad (34)$$

$$\varrho^*Da\overline{v}+\frac{d}{dx}\overline{p}+\varrho^*(\overline{v}-Da)\frac{d}{dx}v^*+\overline{\varrho}(v^*-D)\frac{d}{dx}v^*+\varrho^*(v^*-D)\frac{d}{dx}\overline{v}=0, \quad (35)$$

$$Da\overline{p}+\frac{5}{3}\left(p^*\frac{d}{dx}\overline{v}+\overline{p}\frac{d}{dx}v^*\right)+(v^*-D)\frac{d}{dx}\overline{p}+(\overline{v}-Da)\frac{d}{dx}p^*=\frac{Q_R^\star Dt_c\overline{\tau}_A}{3}. \quad (36)$$

Linear stability - Modeling

The linearized reaction rates:

$$\begin{aligned}
\overline{\tau}_B &= -\overline{\tau}_A, \\
\overline{\tau}_A &= -4d_r^2\sqrt{\tfrac{\pi k}{m}}e^{-\epsilon^\star}\left[\left(2n_A^*\overline{n}_A\sqrt{T^*}+\frac{\overline{p}+\frac{\overline{n}}{n^*}p^*}{2n^*k\sqrt{T^*}}\,{n_A^*}^2\right)\right. \\
&\qquad \left.\left(1+\epsilon^\star+\Gamma{x_A^*}^2\right)+2\sqrt{T^*}\,\frac{{n_A^*}^3}{n^*}\left(-n_A^*\overline{n}_B+n_B^*\overline{n}_A\right)\right],
\end{aligned} \tag{37}$$

where

$$\Gamma=\frac{1}{128}\left(\frac{d}{d_r}\right)^2 Q_R^\star\left(1+Q_R^\star+Q_R^\star\varepsilon_A^\star+\varepsilon_A^\star-2\varepsilon_A^{\star 2}\right)\left(4\varepsilon_A^{\star 3}-8\varepsilon_A^{\star 2}-\varepsilon_A^\star-1\right)e^{-\varepsilon_A^\star}. \tag{38}$$

- Step 4 (Initial conditions)

Linearize the perturbed Rankine-Hugoniot relations:

$$\overline{n}_\alpha(0) = \frac{(n_\alpha^* - n_\alpha^+)\, a - n_\alpha^* \overline{v}(0)}{v^* - D}\,, \qquad \alpha = A, B, \tag{39}$$

$$\overline{v}(0) = \frac{3\varrho^+ v^{*2} + \frac{3}{2}(p^* - p^+) - \frac{3}{2} D \varrho^+ v^* + 2E_A n^+ + Q_R^* n_B^+}{-\varrho^* (v^* - D)^2 + \frac{5}{2} p^*}\, a\,, \tag{40}$$

$$\overline{p}(0) = -\varrho^+ a v^* - (v^* - D)\, \varrho^* \overline{v}(0)\,. \tag{41}$$

Linear stability - Modeling

Problem: The system is not closed.
It is necessary an additional boundary condition:

$$\overline{v}(x_F) + a = \frac{-1}{\gamma \varrho^*_{eq} c^*_{eq}} \overline{p}(x_F), \tag{42}$$

where γ is the ratio of specific heats, c^*_{eq} and ϱ^*_{eq} the isentropic sound speed and mixture mass density at $x = x_F$.

Linear stability - Numerical procedure

The zeros of the function $\mathcal{H}$ defined by

$$\mathcal{H}(a) = \overline{v}(x_F) + a + \frac{1}{\gamma \varrho^*_{eq} c^*_{eq}} \overline{p}(x_F)\,, \quad a \in \mathcal{R} \subset \mathbb{C}, \tag{43}$$

satisfy the boundary condition (42).

The parameter a is used as a trial value in the stability governing equations (33–36) with initial conditions given by (39–41). Two things can happen:

- a is a zero of $\mathcal{H}$ and we have a stability problem solution;
- a is not a zero of $\mathcal{H}$ and we do not have a stability problem solution.

Linear stability - Numerical procedure

If a is a stability problem solution then:

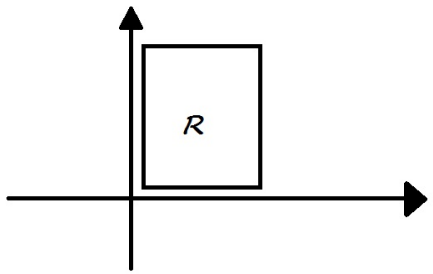
- If $\mathrm{Re}\, a > 0$ then the solution is unstable;
- If $\mathrm{Re}\, a < 0$ then the solution is stable.

A steady solution is:

- Stable if all the stability problem solutions are stable;
- Unstable if at least one of the stability problem solutions is unstable.

Linear stability - Numerical procedure

Problem: Search for unstable solutions (modes) in the complex plan.



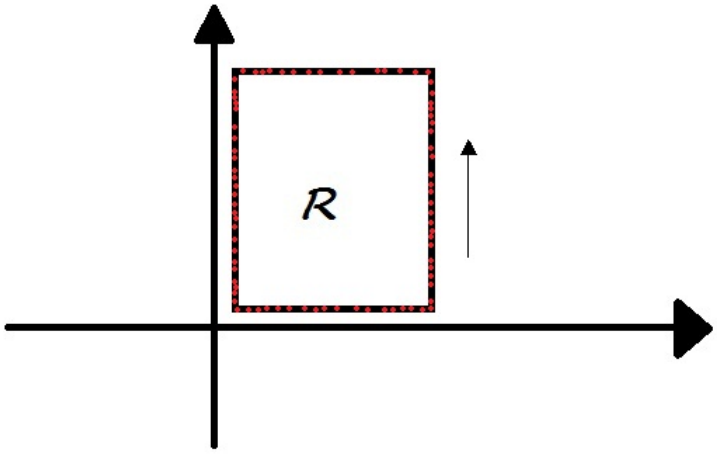
Count the number of zeros of $\mathcal{H}$ in region $\mathcal{R}$ using the argument principle also used by Erpenbeck:

$$Z - P = \frac{1}{2\pi i} \int_k^\ell \frac{\mathcal{H}'(\zeta(t))}{\mathcal{H}(\zeta(t))} \parallel \zeta'(t) \parallel dt, \tag{44}$$

where $\zeta : [k, \ell] \to \mathbb{C}$ is a path smooth by parts, describing the contour of $\mathcal{R}$ in the positive sense.

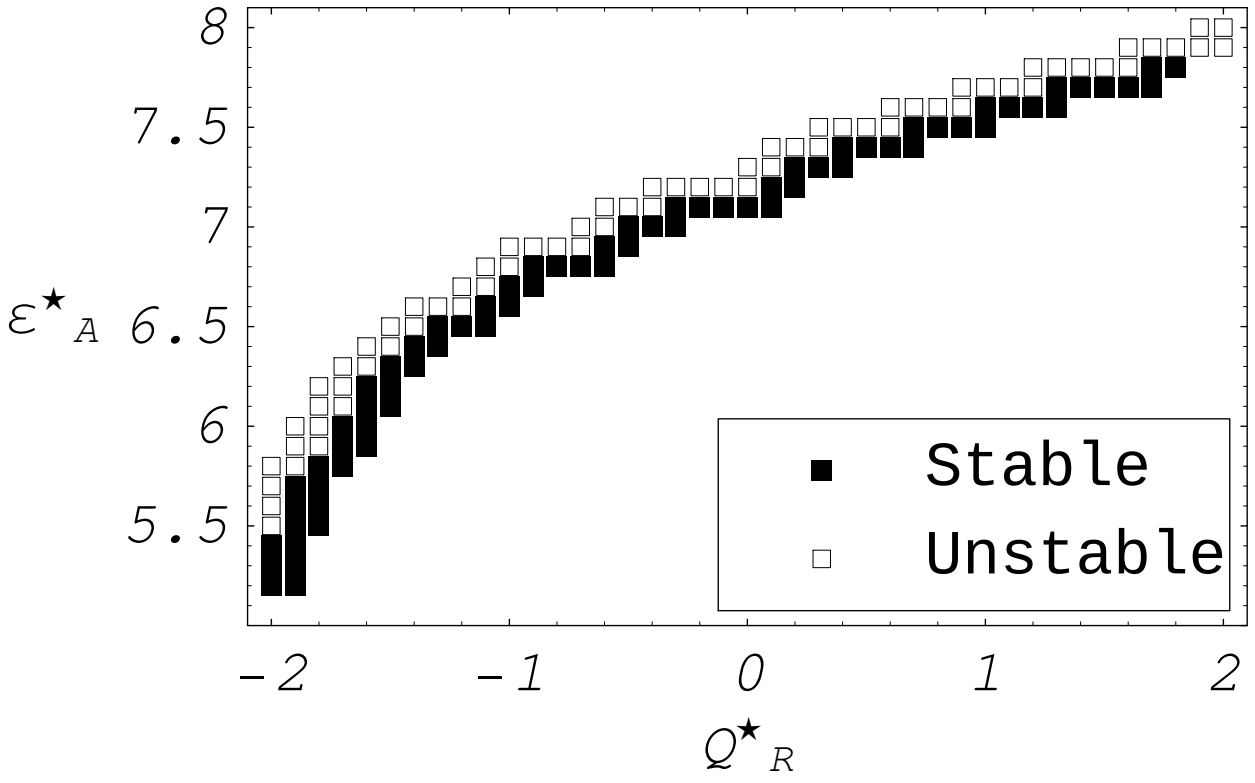
Linear stability - Numerical procedure

Procedure:



1. Choose the domain $\mathcal{R}$;
2. Define a path ζ;
3. Select trial values a_j;
4. Define $b_j = a_j + 10^{-6}$;
5. Solve the stability governing equations (33–36) with initial conditions (39–41) for each point a_j and b_j;
6. Evaluate the residual function $\mathcal{H}$ at each point a_j and b_j;
7. Estimate $\mathcal{H}'(a_j)$ by $\mathcal{H}'(a_j) = (\mathcal{H}(b_j) - \mathcal{H}(a_j))/(b_j - a_j)$;
8. Estimate μ using the mean value of expression $\frac{\mathcal{H}'(\zeta(t))}{\mathcal{H}(\zeta(t))} \parallel \zeta'(t) \parallel$ and a 99% confidence interval;
9. Count the number of zeros: $Z = \frac{1}{2\pi i} \int_k^\ell \frac{\mathcal{H}'(\zeta(t))}{\mathcal{H}(\zeta(t))} \parallel \zeta'(t) \parallel dt = \frac{1}{2\pi i}(k - \ell)\mu.$

Linear stability - Numerical results



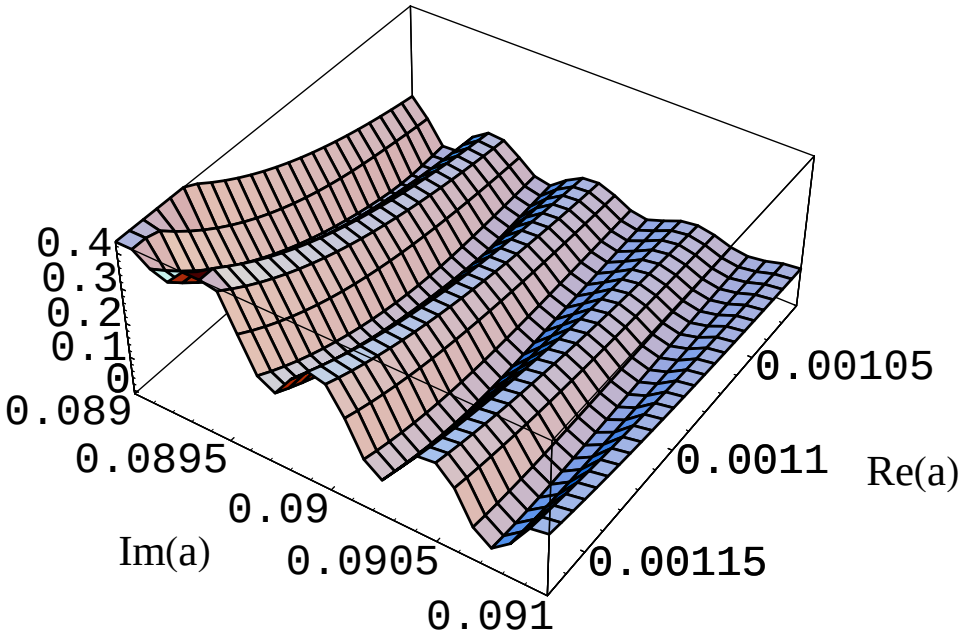
Stability boundary in the $Q^*_R - \varepsilon^\star_A$ plane, for the considered region $\mathcal{R}$.

Linear stability - Numerical results

$Q_R^\star$	number of modes		$Q_R^\star$	number of modes
2	0		-0.62	1
1.5	0		-0.65	2 to 3
1	0		-0.7	4 to 7
0	0		-1	18 to 24
-0.5	0		-1.5	57 to 70
-0.6	0		-2	215 to 252

Number of the instability modes in the domain $\mathcal{R}$, for fixed forward activation energy, $\varepsilon_A^\star = 7$, and different values of the reaction heat in the range $-2 \leq Q_R^\star \leq 2$.

Linear stability - Numerical results



Three-dimensional plot of $|\mathcal{H}(a)|$, in the sub-domain of $\mathcal{R}$ defined by $Re\,(a) \in [0.00102, 0.00117]$, $Im\,(a) \in [0.089, 0.091]$, for $Q_R = -0.1$ and $\varepsilon_A^\star = 7.5$.

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