# DETONATION WAVE PROBLEMS: MODELING, NUMERICAL SIMULATIONS AND LINEAR STABILITY

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Abstract. Traveling waves arising in detonation physics are described by the reactive Euler equations obtained in the fluid dynamical limit of the Boltzmann equation for a binary reactive mixture. The hydrodynamic linear stability of the detonation wave solution is investigated with a normal mode analysis. Numerical simulations are performed for both the detonation wave solution and its linear stability.

1. **Introduction.** Detonation waves are combustion fronts triggered by a strong shock and sustained by a chemical reaction [1, 2]. They can be mathematically modeled by the reactive Euler equations, which includes conservation laws of momentum and total energy (kinetic and chemical) of the mixture as well as reaction rate equation for the constituents. Experimental studies show that the detonation waves tend to be structurally unstable and a first attempt to understand and describe the instabilities is a hydrodynamic stability analysis based on the linearization of the governing Euler equations and a normal-mode representation of the perturbations [3]. It is well known that the numerical analysis of detonation waves and its hydrodynamic stability is a rich and challenging problem with many engineering applications [2, 3]. We investigate this problem starting by considering a binary mixture modeled by the Boltzmann equation for the constituent distribution functions, with both elastic scattering and reactive collision terms. Then we pass to the fluid dynamical limit for an Eulerian regime and use the resulting macroscopic reactive equations to investigate the existence of detonation wave solutions. The analysis presented in this paper includes the modeling of the detonation waves, its hydrodynamic stability and the numerical treatment of these problems.

2. **The model for the explosive reactive mixture.** We consider an idealized explosive mixture of two constituents, denoted by A and B, whose particles undergo a reversible symmetric chemical reaction of type A + A ⇌ B + B. The molecules have binding energies $E_A$ and $E_B$, the same mass $m$ and equal diameter d.

In one-space dimension, the macroscopic physical observables of the reactive mixture are the constituent number densities $n_A$, $n_B$, the mixture mean velocity $v$ and the mixture temperature $T$. Neglecting diffusion and heat fluxes, as well as shear and non-equilibrium stresses, the governing equations of the mixture are the reactive Euler equations, namely the rate equations of the constituents together with the conservation laws of momentum and total energy of the whole mixture. They are given by

$$\frac{\partial n_\alpha}{\partial t} + \frac{\partial}{\partial x}(n_\alpha v) = \tau_\alpha, \qquad \alpha = A, B \tag{1}$$

$$\frac{\partial}{\partial t}(\varrho v) + \frac{\partial}{\partial x}(\varrho v^2 + p) = 0 \tag{2}$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\varrho v^2 + \frac{3}{2}nkT + n_A E_A + n_B E_B\right) \tag{3}$$
$$+ \frac{\partial}{\partial x}\left[pv + \left(\frac{1}{2}\varrho v^2 + \frac{3}{2}nkT + n_A E_A + n_B E_B\right)v\right] = 0$$

where $\tau_\alpha$ represents the reaction rate of the $\alpha-$constituent, such that $\tau_B = -\tau_A$ as predicted by the chemical law. Moreover, $\varrho$, $p$ and $n$ are the mass density, pressure and number density of the whole mixture, with

$$n = n_A + n_B, \qquad \varrho = mn, \qquad p = nkT \tag{4}$$

The number density $n_\alpha$ represents a measure of the concentration of the constituent $\alpha$ and thus Eq. 1 constitutes the rate equation of the considered reactive mixture. The term $n_A E_A + n_B E_B$ appearing in Eq. 3 represents the chemical bond energy of the mixture, and $k$ is the Boltzmann constant.

The above governing equations 1-3 have been derived from a kinetic theory based on the Boltzmann equation extended to the considered reactive mixture, see Ref. [4, 5]. In particular, a chemical regime of slow reactive process is assumed and an appropriate scalling is introduced in terms of the Knudsen number associated to elastic scattering. The corresponding fluid dynamic limit is obtained by means of the Chapman-Enskog method [6] which leads to a distribution function containing the non-equilibrium effects associated to the chemical reaction. The procedure leads to the explicit computation of the reaction rate $\tau_\alpha$, which follows an Arrhenius-type law, given by

$$\tau_B = -\tau_A, \quad \tau_A = -4n_A^2 \mathsf{d}_r^2 \sqrt{\frac{\pi kT}{m}}\, e^{-\varepsilon_A^\star}\left[1 + \varepsilon_A^\star + \frac{n_A^2}{128 n^2}\left(\frac{\mathsf{d}}{\mathsf{d}_r}\right)^2 Q_R^\star\right.$$
$$\left. \times \left(1 + Q_R^\star + Q_R^\star \varepsilon_A^\star + \varepsilon_A^\star - 2\varepsilon_A^{\star 2}\right)\left(4\varepsilon_A^{\star 3} - 8\varepsilon_A^{\star 2} - \varepsilon_A^\star - 1\right)e^{-\varepsilon_A^\star}\right] \tag{5}$$

where $\varepsilon_A^\star$ is the activation energy of the forward chemical reaction in units of $kT$ and $Q_R^\star = 2(E_B - E_a)/kT$ is the reaction heat of the chemical reaction, also in units of $kT$. The details of the passage to the fluid dynamic limit are given in Ref. [7] and revisited in Refs. [4, 5].

The qualitative properties of the Euler equations are well known in literature, see for example Refs. [8, 9, 10]. In particular they constitute an hyperbolic set of non-linear PDE's and admit shock profile solutions.

In addition, when a reactive gaseous mixture is considered, like the one previously introduced in this section, an interesting and relevant type of shock solutions may arise, namely steady traveling detonation wave solutions.

3. **Detonation waves.** Physically, detonation wave solutions represent a combustion front in which a strong shock wave ignites the explosive mixture and the burning keeps the shock advancing and proceeding to equilibrium in the reaction zone behind the shock. The configuration of such solutions is well described in the literature of the detonation phenomenon and a good and accepted model for such solutions is the well known ZND model developed by Zeldovich, von Neumann and Doering, the founders of the modern detonation theory, see Refs. [1, 2]. According to the ZND model, the structure of the detonation wave solution consists of a leadind planar non-reactive shock propagating with constant velocity, followed by a finite reaction zone where the chemical process evolves.

3.1. **Steady detonation solutions.** We investigate one-dimensional ZND steady detonation wave solutions propagating in an explosive mixture described by the model of Section 2. Mathematically, these solutions are traveling waves for the reactive Euler equations 1-3.

We consider a planar shock wave propagating in the $x-$direction with constant velocity $D$ from left to the right. Ahead the shock front, we consider the initial quiescent mixture at rest, where the rate of the chemical reaction is negligible. Such *initial state* is labeled as $I = (n_A^+, n_B^+, 0, T^+)$. The passage of the shock raises the density and temperature above the ignition values, so that the chemical reaction is suddenly activated. The state just behind the shock wave, where the chemical reaction is triggered, is the *von Neumann state* which is labeled as $N = (n_A, n_B, v, T)$. The shock wave is followed by a reaction zone with a finite length, where the chemical reaction continuously proceeds from the state $N$ to a *final state* $F$ of chemical equilibrium. All states inside the reaction zone are *intermediate states* $R$ of partial reaction.

Traveling detonation waves with velocity $D$ are determined as solutions depending on the normalized steady variable

$$x_s = \frac{x - Dt}{Dt_c}, \qquad \text{with} \qquad t_c = \frac{1}{4n^+\mathsf{d}^2}\sqrt{\frac{m}{\pi kT^+}} \tag{6}$$

where $t_c$ is a characteristic time. The Euler equations 1-3 are transformed to the steady frame attached to the shock wave and re-written in terms of the variable $x_S$. They transform to a system of four ODE's for the unknowns $n_A, n, v, T$, which can be writen in the more conservative form

$$\frac{d}{dx}\Big[(v - D)\, n_A\Big] = Dt_c\tau_A \tag{7}$$

$$\frac{d}{dx}\Big[(v - D)\, n\Big] = 0 \tag{8}$$

$$\frac{d}{dx}\Big[(v - D)\, \varrho v + nkT\Big] = 0 \tag{9}$$

$$\frac{d}{dx}\left[(v - D)\left(\frac{3}{2}nkT + \frac{\varrho v^2}{2} + E_A n_A + E_B n_B\right) + nkTv\right] = 0 \tag{10}$$

where we have written $x$ in place of $x_S$. The explicit expression of the reaction rate is given by expression 5.

*Von Neumann state.* State $N$, just behind the shock wave, is the solution of a non-reactive shock problem. Euler equations 7-10 hold true with vanishing reaction rate and should be taken in a weak integrated sense between the initial state and the von Neumann state. The integration leads to the algebraic Rankine-Hugoniot jump conditions connecting the state $N$ to the state $I$, namely

$$n_A (v - D) = -n_A^+ D \tag{11}$$

$$n (v - D) = -n^+ D \tag{12}$$

$$\varrho v (v - D) + nkT = kn^+ T^+ \tag{13}$$

$$\left( \frac{3}{2} nkT + \frac{\varrho v^2}{2} + E_A n_A + E_B n_B \right) (v - D) + nkTv$$
$$= - \left( \frac{3}{2} kn^+ T^+ + E_A n_A^+ + E_B n_B^+ \right) D \tag{14}$$

*Intermediate and final states.* States $R$ and $F$, in the reaction zone, are obtained solving an initial value problem for the number density $n_A$, with initial condition assigned at the von Neumann state. The chemical reaction is the dominant process within this problem since the evolution of the gaseous mixture within the reaction zone is determined by the reactive process. More in detail, conservative Eqs. 8-10 are integrated between the initial state and an arbitrary state within the reaction zone. The resulting three algebraic Rankine-Hugoniot conditions allow to express the state variables $n_B$, $v$ and $T$ in terms of $n_A$ and reduce the system to the ODE

$$\frac{dn_A}{dx} = \frac{Dt_c \tau_A}{v - D + n_A \frac{dv}{dn_A}} \tag{15}$$

Equation 15 represents the rate law in the shock attached frame and specifies the chemical composition of the explosive mixture in the reaction zone. The integration of Eq. 15 and further computation of the remaining state variables through the three algebraic Rankine-Hugoniot conditions characterize the thermodynamical state of the mixture in the reaction zone. The final state of chemical equilibrium, is obtained when the reaction rate $\tau_A$ vanishes and $n_A$ becomes constant, so that the chemical concentrations of constituents A and B remain unchanged.

3.2. **Numerical solutions.** Numerical solutions of the detonation wave problem can be determined, characterizing the states $N$, $R$ and $F$ for different values of the velocity $D$, reaction heat $Q_R^*$ and activation energy $\varepsilon_A^\star$. Some numerical simulations are performed for one elementary reaction of a theoretical detonating mixture. The initial state are assumed as follows

$$m = 0.01 \, Kg/mol, \quad n_A^+ = 0.35 \, mol/l, \quad n_B^+ = 0 \, mol/l$$
$$T^+ = 298.15 \, K, \quad E_A = 2400 \, K, \quad \varepsilon_A^\star = 6 \tag{16}$$

Some representative profiles are shown in Figure 1 for the mixture pressure, in dependence of the algebraic distance behind the shock wave. The left frame of Figure 1 is obtained for a fixed detonation velocity and refers to exothermic chemical reactions with reaction heat $Q_R^* = -2$ and $Q_R^* = -1$. It shows that the pressure profile and the thickness of the reaction zone decrease for the hight absolute value of the reaction heat. The right frame refers to exothermic reaction with $Q_R^* = -1$
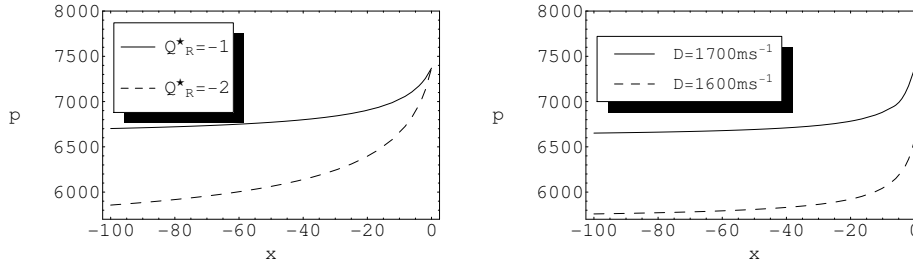
FIGURE 1. Mixture pressure profile. *Left:* detonation velocity $D=1700\,ms^{-1}$, exothermic reaction with $Q_R^\star=-1$ (solid line) and $Q_R^\star=-2$ (dashed line). *Right:* reaction heat $Q_R^\star=-1$ (exothermic reaction), detonation velocity $D=1700\,ms^{-1}$ (solid line) and $D=1600\,ms^{-1}$ (dashed line).

and detonation velocity $D=1600\,ms^{-1}$ and $D=1700\,ms^{-1}$. It shows that the pressure profile increases and the thickness of the reaction zone decreases for the hight value of the detonation velocity. The results are in a good agreement with the analytical studies and numerical predictions known from the literature on the detonation phenomenon. See, for example, Refs. [1, 2]. A more detailed discussion about these results can be seen in Ref. [5].

4. **Hidrodynamic linear stability.** It is well known from theoretical studies and experimental investigations, see Refs. [1, 2], that the detonation wave solution tends to be structurally unstable and can degenerate into an oscillatory solution in the long-time limit. Such oscillatory configuration exhibits complex three-dimensional non-linear perturbations, so that its characterization results to be a very complex and difficult problem, from either analytical or numerical point of view.

As a first step of a formal treatment, one studies the problem of hydrodynamical stability of the steady solution, formulated as follows: one assumes that a small rear boundary perturbation is instantaneously assigned, inducing a deviation on the shock wave position; as a consequence, small perturbations are induced on the state variables and one is interested in their evolution in the reaction zone. The pertinent question is to investigate if all perturbations decay with time or if any perturbation grow with time. In the first case, the steady solution becomes stable and in the latter it becomes unstable.

4.1. **Stability analysis.** From the mathematical point of view, the stability problem requires first the transformation to the perturbed wave coordinate

$$\overline{x} = x - \psi(t), \qquad \text{with} \qquad \psi(t) = Dt + \widetilde{\psi}(t) \tag{17}$$

where $\psi(t)$ represents the location of the perturbed shock wave and $\widetilde{\psi}(t)$ the displacement of the wave from the unperturbed position.

*Normal mode approach.* Since the perturbations are small, we then linearize the governing equations and Rankine-Hugoniot conditions about the steady detonation solution, assuming the following expansions for the the state variables and shock distortion with exponential time dependence,

$$z(x,t) = z^*(x) + e^{at}\,\overline{z}(x), \qquad \psi(t) = e^{at}, \qquad a \in \mathbb{C} \tag{18}$$

where $z = [n_A \; n_B \; v \; p]^T$, $z^*(x)$ is the steady solution, $\overline{z}(x)$ is the vector of complex eigenfunctions representing the unknown spatially disturbances, and $a$ is the complex eigenvalue, with $\mathrm{Re}\, a$ and $\mathrm{Im}\, a$ being the disturbance growth rate and frequency, respectively.

*Linearized stability equations.* The transformation to the perturbed shock and the linearization by means of the expansions 18 lead to the stability equations

$$Da\overline{n}_\alpha + (v^* - D)\frac{d\overline{n}_\alpha}{dx} + \frac{dn_\alpha^*}{dx}(\overline{v} - aD) + \frac{dv^*}{dx}\overline{n}_\alpha + n_\alpha^*\frac{d\overline{v}}{dx} = \overline{\tau}_\alpha, \quad \alpha = A, B \qquad (19)$$

$$\varrho^* aD\overline{v} + \frac{d\overline{p}}{dx} + \varrho^*\frac{dv^*}{dx}(\overline{v} - aD) + (v^* - D)\frac{dv^*}{dx}\overline{\varrho} + \varrho^*(v^* - D)\frac{d\overline{v}}{dx} = 0 \qquad (20)$$

$$Da\overline{p} + \frac{5}{3}\left(p^*\frac{d\overline{v}}{dx} + \overline{p}\frac{dv^*}{dx}\right) + (v^* - D)\frac{d\overline{p}}{dx} + (\overline{v} - aD)\frac{dp^*}{dx} = \frac{Q_R^* Dt_c\overline{\tau}_A}{3} \qquad (21)$$

where the linearized reaction rate $\overline{\tau}_\alpha$ is given by

$$\overline{\tau}_A = -4\mathsf{d}_r^2\sqrt{\frac{\pi k}{m}}e^{-\epsilon^\star}\left[\left(2n_A^*\overline{n}_A\sqrt{T^*} + \frac{\overline{p} + \frac{\overline{n}}{n^*}p^*}{2n^* k\sqrt{T^*}}n_A^{*\,2}\right)\left(1 + \epsilon^\star + \Gamma x_A^{*\,2}\right)\right.$$

$$\left. + 2\sqrt{T^*}\frac{n_A^{*\,3}}{n^*}\left(-n_A^*\overline{n}_B + n_B^*\overline{n}_A\right)\right], \qquad \overline{\tau}_B = -\overline{\tau}_A$$

Equations 19-21 constitute a system of eight first-order homogeneous linear ordinary differential equations with spatially varying coefficients, for the real and imaginary parts of the complex perturbations.

*Initial conditions.* The initial conditions for the stability equations are obtained from the Rankine-Hugoniot relations 11-14, after transforming to the wave coordinate and linearizing around the steady state. The resulting conditions are

$$\overline{n}_\alpha(0) = \frac{(n_\alpha^* - n_\alpha^+)a - n_\alpha^*\overline{v}(0)}{v^* - D}, \qquad \alpha = A, B \qquad (22)$$

$$\overline{v}(0) = \frac{3\varrho^+ v^{*\,2} + \frac{3}{2}(p^* - p^+) - \frac{3}{2}D\varrho^+ v^* + 2E_A n^+ + Q_R^* n_B^+}{-\varrho^*(v^* - D)^2 + \frac{5}{2}p^*}a \qquad (23)$$

$$\overline{p}(0) = -\varrho^+ av^* - (v^* - D)\varrho^*\overline{v}(0) \qquad (24)$$

*Closure condition.* Equations 19-21 and their initial conditions 22-24 involve the complex perturbation parameter $a$ and therefore the stability system is not closed. The closure condition is given by the dispersion relation of the normal modes 18 formulated at the final state $F$, that is

$$\overline{v}_F + a = \frac{-1}{\gamma\varrho_{eq}^* c_{eq}^*}\overline{p}_F, \qquad (25)$$

where $\gamma$ is the ratio of specific heats, $c_{eq}^*$ and $\varrho_{eq}^*$ the isentropic sound speed and gas density at the equilibrium final state.

*Stability problem.* The linear stability problem consists in the *eight* ordinary differential equations 19-21 for the complex eigenfunction disturbances $\overline{z}(x)$ and complex eigenvalue parameter $a$, with initial conditions 22-24 and closure condition 25.

The objective is to determine the instability modes which correspond to a positive growth rate $\mathrm{Re}\, a$. Moreover, since these modes occur in conjugate pairs, they are searched in the upper-right quarter of the complex plane.

The stability problem is solved numerically and its solution gives valuable predictions about the stability of the steady detonation solutions.

4.2. **Numerical technique.** For a given set of thermodynamical and chemical parameters characterizing the steady detonation wave solution, eigenfunctions $\overline{z}(x)$ and eigenvalues $a$ are determined. We apply a numerical technique which combines the iterative shooting method proposed by Lee and Stewart in paper [3] with the argument principle used by Erpenbeck in paper [11]. The basic idea is the following, see Ref. [5]: *(i)* we start with a trial value of $a$ in a fixed bounded domain $\mathcal{R}$ of the complex plane; *(ii)* then we use a fourth order Runge-Kutta routine to integrate the stability equations 19-21 in the reaction zone, say for $x \in ]x_F, 0[$, with initial conditions 22-24 at $x = 0$; *(iii)* finally we enquire if the approximate solution $\overline{z}(x)$, $x \in ]x_F, 0]$ and related parameter $a$ satisfy the boundary condition 25; *(iv)* if this is not the case, we iterate the procedure on the trial value $a$ until condition 25 is satisfied. Since, in general, a trial value of $a$ does not produce a stability solution, in the sense that condition 25 is not verified, the key preliminary step consists in searching appropriate trial values for $a$. To do this, we introduce the residual function

$$\mathscr{H}(a) = \overline{v}(x_F) + a + \frac{1}{\gamma \varrho_{eq}^* c_{eq}^*} \, \overline{p}(x_F), \quad a \in \mathcal{R}, \tag{26}$$

and search the zeros of $\mathscr{H}$ in the considered region $\mathcal{R}$. To count the number $Z$ of zeros we use the argument principle and estimate the quantity

$$Z = \frac{1}{2\pi i} \int_k^\ell \frac{\mathscr{H}'(\zeta(t))}{\mathscr{H}(\zeta(t))} \, \| \zeta'(t) \| \, dt \tag{27}$$

where $\zeta : [k, \ell] \to \mathbb{C}$ is a path smooth by parts, describing the contour of $\mathcal{R}$ in the positive direction. Such estimation requires a rather involved numerical technique which is explained in detail in Refs. [4, 5]. Finally successive refinements of $\mathcal{R}$ are considered and a three-dimensional plot of $|\mathscr{H}|$ in the last refinement is used to determine the location of the zeros.

Some numerical simulations are performed in order to investigate the response of the steady detonation wave solution to the rear boundary perturbations.

4.3. **Stability results.** The stability problem is solved numerically for the set of thermodynamical and chemical parameters given in Eq. 16. We choose a rectangular region $\mathcal{R}$ in the upper-right complex plane such that $0.001 < Re(a) < 0.02$ and $0.001 < Im(a) < 0.1$. The reaction heat and the detonation velocity are varying in the ranges $-2 \leq Q_R^* \leq 2$ and $1278\,ms^{-1} \leq D \leq 1896\,ms^{-1}$, respectively. Table 1 shows the number of instability modes in the region $\mathcal{R}$, for different values of the detonation velocity, and for fixed reaction heat and activation energy, $Q_R^\star = -1$ and $\varepsilon^\star = 6.5$. One can see that the number of instability modes in the region $\mathcal{R}$ is zero when $D \geq 1645\,ms^{-1}$, and that it increases for lower values of $D$.

| Detonation velocity | Number of modes | Detonation velocity | Number of modes |
|---|---|---|---|
| $1896\,ms^{-1}$ | 0 | $1518\,ms^{-1}$ | 17 to 28 |
| $1700\,ms^{-1}$ | 0 | $1391\,ms^{-1}$ | 57 to 120 |
| $1645\,ms^{-1}$ | 0 | $1328\,ms^{-1}$ | 250 to 334 |
| $1581\,ms^{-1}$ | 1 to 3 | $1278\,ms^{-1}$ | 442 to 493 |

TABLE 1. Number of instability modes in the region $\mathcal{R}$, for different values of the detonation velocity $D$. The reaction is exothermic with reaction heat $Q_R^\star = -1$ and activation energy $\varepsilon^\star = 6.5$.

Figure 2 shows the stability boundary in the parameter plane $Q_R^* - \varepsilon_A^\star$, for detonation velocity $D = 1700 \, ms^{-1}$. A pair $(Q_R^*, \varepsilon_A^\star)$ in the stability zone indicates that for the corresponding values of $Q_R^*$ and $\varepsilon_A^\star$, no instability modes have been found in the domain $\mathcal{R}$. Conversely, a pair in the instability zone indicates that one instability mode, at least, has been found in $\mathcal{R}$.
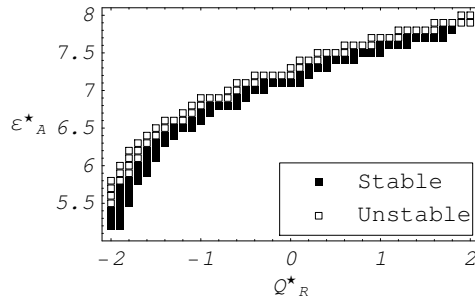


FIGURE 2.   Stability boundary in the $Q_R^\star - \varepsilon^\star$ plane, for detonation velocity $D = 1700 \, ms^{-1}$ and for the considered region $\mathcal{R}$.

The results of Table 1 can be compared to those of Figure 2 considering, simultaneously, $Q_R^\star = -1$, $\varepsilon^\star = 6.5$ and $D = 1700 \, ms^{-1}$. The results in both representations indicate a stable solution since no instability modes are found.

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