A Kinetic Approach to Steady Detonation Waves and Their Linear Stability

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Abstract Detonation waves have a relevant role in many engineering processes, namely those related to propulsion. Most studies, regarding the stability of detonation waves, have been carried out by computer simulations, notwithstanding their multi-scale nature and unstable behaviour makes it difficult to achieve accurate results. In this paper we propose a kinetic approach to this problem, explain the constraints and the difficulties that this choice entails as well as its advantages. Numerical methods are needed to obtain the solutions of the stability. The ones in use imply that a regular computer takes a long period of time to provide the solutions. In this paper, taking into account the developments proposed by others, we present a numerical procedure that helps to overcome the difficulties of the current methods and allows us to answer some questions related to the stability problem.

Keywords Kinetic theory · Boltzmann equation · Chemical reactions
Steady detonation waves · Hydrodynamic stability

1 Introduction

In kinetic theory of gases the description of a gas system evolution is obtained using distribution functions in the mesoscopic level. These distributions are defined in the phase space composed by the position x, and the velocity c for a given time t in such a way that $f(x, c, t)$ represents the number of particles that, at time t, are in the volume element $dxdc$ around position x and velocity c.

The basic assumption of kinetic theory modelling is that the number of particles of a gas is so large that it can be treated as a continuum. If we consider that particles obey

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classical laws of mechanics and we neglect macroscopic forces acting on the particles and interactions between them, according to Newton's Principle, each particle travels at constant velocity along a straight line, therefore, $f(x, c, t) = f(x - ct, c, 0)$ for any time t. In these conditions, f is a weak solution of the free transport equation

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} c_i \frac{\partial}{\partial x_i} f = 0. \tag{1}$$

In 1872, see Ref. [1] Ludwig Boltzmann derived an equation, the so called Boltzmann Equation, that is used to describe the evolution of a gas, considering that particles interact. This derivation was based on some physical assumptions (for more details see for instance [1] or [2]):

(a) the collision time is much smaller in comparison with the free travelling time of a particle;
(b) collisions between more than two particles may be neglected;
(c) collisions are micro-reversible;
(d) the velocities of two particles that are about to collide are uncorrelated;
(e) there are some physical quantities that do not change during a collision, such as mass, linear momentum and kinetic energy.

The Boltzmann Equation is an integro-differential equation that, considering a single gas specie without macroscopic forces acting on the particles, has the following expression [3]:

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} c_i \frac{\partial}{\partial x_i} f = \mathcal{Q}(f, f), \tag{2}$$

where $\mathcal{Q}(f, f)$ is the integral collisional operator. An extension of the Boltzmann equation to chemical reactive gases, will be presented with more detail in the next section.

The Boltzmann Equation was then extended to many different situations, such as gases with macroscopic forces acting on the particles, gases with more than one constituent, gases with more than one constituent where particles may interact not only in elastic collisions but also in reactive collisions, polyatomic gases, relativistic systems, among others.

The equilibrium solution is the only exact solution of the Boltzmann Equation, that is currently known. The wide range of applications of this equation and the difficulties of finding its solutions led many researchers to develop simplified variants of the Boltzmann equation which allowed them to find solutions, while still retaining its main features. The BGK model [4], the Kac model [5] and the discrete-velocity models [6] are some of the examples. Others, such as Grad, Chapman and Enskog, developed different methods to obtain approximate solutions of the full Boltzmann Equation.

In this work we will address the problem of the detonation wave propagation, that will be presented in Sect. 3 and its stability analysis that will be presented in Sect. 4. The kinetic approach to this problem, using the Boltzmann equation to describe the evolution of the gas system, allows a discussion around the microscopic features of the gas, such as the molecular potential, the reaction heat of the considered chemical reaction and the activation energy needed for the reaction to occur. It also allows the study on their influence in different macroscopic regimes, such as different detonation velocities and different initial concentrations of the gas constituents.

In what follows, we will present some of our work on this subject and make reference to a few other works that were important in the development of the current state of art. The paper is organized as follows. The kinetic description of the gas system is presented in Sect. 2. In Sects. 3 and 4 we present the detonation wave problem and the stability analysis modelling. Finally, in Sect. 5 we discuss some numerical techniques that were used to obtain solutions for the stability analysis and present recent developments on the study of stability.

2 Kinetic Framework and Macroscopic Equations

In this section we present the main microscopic features of the gas system and synthetically explain how to go from the microscopic description to the macroscopic equations that describe the gas evolution.

2.1 Microscopic Modelling

We consider a binary gaseous mixture whose constituents, A and B, have equal molecular mass m and binding energies E_A and E_B. Vibrational and rotational molecular degrees of freedom are not taken into account. The gas particles can undergo binary elastic collisions as well as collisions with chemical reaction according to the single reversible symmetric law

$$A + A \rightleftharpoons B + B. \tag{3}$$

At the mesoscopic scale, the thermodynamical behaviour of the mixture is modelled by the following system of Boltzmann equations for the constituent distribution functions $f_\alpha(x, c_\alpha, t)$, with $x, c_\alpha \in \mathbb{R}^3$ and $t \in \mathbb{R}^+$,

$$\frac{\partial f_\alpha}{\partial t} + c_\alpha \nabla_x f_\alpha = \mathcal{Q}(f_\alpha, f_\alpha), \qquad \alpha = A, B, \tag{4}$$

where $\mathcal{Q}(f_\alpha, f_\alpha) = \mathcal{Q}_\alpha^E + \mathcal{Q}_\alpha^R$, and

$$\mathcal{Q}_\alpha^E = \sum_{\beta=A}^{B} \int \left(f'_\alpha f'_\beta - f_\alpha f_\beta\right) \mathrm{d}^2\left(g_{\beta\alpha} \cdot \mathbf{k}_{\beta\alpha}\right) d\mathbf{k}_{\beta\alpha} d\mathbf{c}_\beta, \tag{5}$$

$$\mathscr{Q}_\alpha^R = \int \left[f_\beta f'_\beta - f_\alpha f'_\alpha \right] \sigma_\alpha^{\star 2} \left(g_\alpha \cdot \mathbf{k}_\alpha \right) d\mathbf{k}_\alpha d\mathbf{c}'_\alpha. \tag{6}$$

Above, in Eq. (5), the primes denote post collisional distribution functions, d the elastic particle diameter, $g_{\beta\alpha}$ the relative velocity between the α and β particles, $\mathbf{k}_{\beta\alpha}$ the unit collision vector and $d\mathbf{k}_{\beta\alpha}$ the element of solid angle for elastic collisions and in Eq. (6), the primes are used to distinguish two identical particles that participate in the reactive collision, $\mathbf{k}_\alpha$ is the unit collision vector, g_α the relative velocity between two identical particles of constituent α, with $(\alpha, \beta) \in \{(A, B), (B, A)\}$, $d\mathbf{k}_\alpha$ the element of solid angle for reactive collisions, and the term $\sigma_\alpha^{\star 2}$ is the differential reactive cross section.

The collisional operator $\mathscr{Q}(f_\alpha, f_\alpha)$, was used by Boltzmann to introduce the influence of the encounters between particles in the description of the evolution of the gas system. In the considered kinetic framework, this operator must consider elastic and reactive collisions, therefore, it is split into two operators: the elastic operator $\mathscr{Q}_\alpha^E$ and the reactive operator $\mathscr{Q}_\alpha^R$. As we can see in Eq. (5), in the elastic operator all collisions are considered, even those between two constituents A or two constituents B that end up being reactive and thus considered in the reactive operator. This double counting shouldn't create any major problem in situations where the number of elastic encounters is much larger than the number of reactive encounters. Although this is what happens more frequently, some recent works introduced a correction term to avoid this problem, see for instance [7].

In what follows, the reactive cross section $\sigma_\alpha^{\star 2}$ is defined as

$$\sigma_\alpha^{\star 2} = \begin{cases} 0 & \text{for } \gamma_\alpha < \varepsilon_\alpha^\star \\ d^2 & \text{for } \gamma_\alpha > \varepsilon_\alpha^\star \end{cases} \quad \alpha = A, B, \tag{7}$$

where the relative translational energy $\gamma_\alpha = \frac{m g_\alpha^2}{4kT}$ and the activation energies $\varepsilon_\alpha^\star$ are written in units of kT, with k being the Boltzmann constant and T the temperature of the mixture. There are many works on reacting gases that choose different collision potential. For more details on the implications of these choices see for instance [3].

2.2 Hydrodynamical Limit

Macroscopic state variables may be defined as mean values of microscopic quantities. For instance, the number densities n_α of the constituents, the mean velocity components v_i and temperature T of the mixture, may be defined by

$$n_\alpha = \int f_\alpha dc_\alpha, \qquad v_i = \frac{1}{n} \sum_{\alpha=A}^{B} \int c_i^\alpha f_\alpha dc_\alpha, \qquad T = \frac{m}{3kn} \sum_{\alpha=A}^{B} \int (c_\alpha - \mathbf{v})^2 f_\alpha dc_\alpha, \tag{8}$$

respectively.

As was explained before, there are some physical microscopic quantities that must be preserved during a collision and a proper microscopic model must respect those physical characteristics. It is possible to prove that the model that is used in this paper has the desired properties. Therefore, if f_α is a solution of the Boltzmann equation, and $\Phi_\alpha \in \left\{1, m_\alpha, m_\alpha c_1^\alpha, m_\alpha c_2^\alpha, m_\alpha c_3^\alpha, \frac{1}{2} m_\alpha c_\alpha^2 + E_\alpha\right\}$ then, multiplying both sides of the Boltzmann equation (2.1) by the proper Φ_α and integrating over c_α leads to the following macroscopic equations

$$\frac{\partial n_\alpha}{\partial t} + \sum_{i=1}^{3} \frac{\partial n_\alpha}{\partial x_i} \left(n_\alpha v_i + n_\alpha u_i^\alpha\right) = \tau_\alpha, \tag{9}$$

$$\frac{\partial}{\partial t}(\rho v_i) + \sum_{j=1}^{3} \frac{\partial}{\partial x_i} \left(p_{ij} + \rho v_i v_j\right) = 0, \tag{10}$$

$$\frac{\partial}{\partial t}\left(\frac{3}{2} nkT + \sum_{\alpha=A}^{B} n_\alpha E_\alpha + \frac{1}{2}\rho v^2\right) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left\{q_i + \sum_{j=1}^{3} p_{ij} v_j + \left(\frac{3}{2} nkT + \sum_{\alpha=A}^{B} n_\alpha E_\alpha + \frac{1}{2}\rho v^2\right) v_i\right\} = 0. \tag{11}$$

Above, u_i^α and τ_α are the diffusion velocity components and the reaction rate of the constituent α, and ρ, p_{ij}, q_i are the mass density, pressure tensor and heat flux of the gas system.

These six Eqs. (9)–(11) do not form a closed system and we must pass to the hydrodynamic limit to close it. Here we adopt the solution obtained in [8] using the asymptotic method of Chapman-Enskog and a second order Sonine expansion of the distribution functions. This approximate solution was used to describe the complete reactive process, starting from its early stage and going towards the equilibrium final state. Depending on the chemical regimes that we want to model, we may consider other regimes or even other approximation methods. In paper [9], for example, the author derived a different hydrodynamical limit where elastic encounters are the dominant interactions between particles. The subject of deriving hydrodynamical limits from microscopic descriptions is a research area for itself, see for instance [10, 11]. Although interesting, this subject will not be addressed here.

With the distribution function obtained in [8] we may evaluate some macroscopic quantities of Eqs. (9)–(11) such as the reaction rate τ_α, constituent diffusion velocities u_i^α, mixture pressure tensor p_{ij} and heat flux q_i. The resulting equations, in the one dimensional form, may be rearranged in the following way:

$$\frac{\partial n_A}{\partial t} + \frac{\partial}{\partial x}(n_A v) = \tau_A\,, \tag{12}$$

$$\frac{\partial}{\partial t}(n_A + n_B) + \frac{\partial}{\partial x}\Big[(n_A + n_B)v\Big] = 0, \tag{13}$$

$$\frac{\partial v}{\partial t} + \frac{1}{\rho}\frac{\partial p}{\partial x} + v\frac{\partial v}{\partial x} = 0, \tag{14}$$

$$\frac{\partial p}{\partial t} + v\frac{\partial p}{\partial x} + \frac{5}{3}p\frac{\partial v}{\partial x} + \frac{2}{3}\sum_{\alpha=A}^{B} E_\alpha \tau_\alpha = 0, \tag{15}$$

where v represents now the x-component of the gas system velocity. This choice was motivated by the fact that these equations' aim is to study the one dimensional detonation wave. This subject is the main topic of the next section.

3 One Dimensional Steady Detonation

The one dimensional detonation wave model is based on the assumption that ahead of a shock there is a gas system in a meta stable equilibrium. This means that in this location, chemical reactions between particles may be neglected but, if a trigger appears, such as a shock wave with a large velocity, then a chemical reaction occurs until the gas system reaches total, elastic and chemical, equilibrium. This phenomenon may be described by the simple ZND (Zel'dovich, John Von Neumann and Werner Döring) model in the case of a detonation wave with velocity greater then the CJ (Chapman-Jouguet) velocity. For more detail see for instance [12, 13].

Many researchers developed studies concerning the detonation wave problem. In paper [14] the authors did so by exploring the reaction zone thickness for different wave velocities and different activation energies. In [15] the influence of the chemical reaction velocity in the detonation wave profiles was studied.

In paper [16], in collaboration with Ana Jacinta Soares, we studied the influence of the reaction heat on the detonation wave profiles and its relation with the activation energy of the chemical reaction. We considered the gas system described before with the chemical reaction defined in Eq. (3) and with the governing Eqs. (12)–(15). Then, transforming these equations' frame to the shock front we obtained the steady state equations:

$$\frac{d}{dx}\Big[(v-D)\,n_A\Big] = D\tau_A, \tag{16}$$

$$\frac{d}{dx}\Big[(v-D)\,(n_A+n_B)\Big] = 0, \tag{17}$$

$$\frac{d}{dx}\Big[(v-D)\,\rho v + nkT\Big] = 0, \tag{18}$$

$$\frac{d}{dx}\left[(v-D)\left(\frac{3}{2}nkT + \frac{\rho v^2}{2} + E_A n_A + E_B n_B\right) + nkTv\right] = 0. \tag{19}$$

These equations with the Rankine-Hugoniot conditions

$$(v - D)\, n_A = -D n_{A0}, \tag{20}$$

$$(v - D)\, n_B = -D n_{B0}, \tag{21}$$

$$(v - D)\, \rho v + nkT = n_0 k T_0, \tag{22}$$

$$(v - D)\left(\frac{3}{2} nkT + \frac{\rho v^2}{2} + E_A n_A + E_B n_B\right) + nkTv = \\ = -D\left(\frac{3}{2} n_0 k T_0 + E_A n_{A0} + E_B n_{B0}\right), \tag{23}$$

constitute a closed equation system that is used to obtain the steady state detonation wave solution for a given set of parameters such as the initial values for the macroscopic variables noted with the subscript 0 and the detonation wave velocity D.

With this system it was possible to observe, for the input parameters, that for an exothermic reaction the steady detonation solution is a rarefaction wave, which means that the pressure decreases along the reaction zone, and for an endothermic reaction the steady detonation solution is a compression wave, which means that the pressure increases along the reaction zone. In addition, it was also possible to observe, among other expected and essential physical features, that the temperature increases for an exothermic chemical reaction and decreases for an endothermic reaction and that the extent of the reaction zone decreases when the reaction heat increases.

These are examples of works where the authors started from a kinetic description of the gas to analyse, using an appropriate hydrodynamic limit, the behaviour of the detonation wave for different values of hider microscopic, such as the reaction heat and activation energy, or macroscopic variables, such as initial concentrations and wave velocity. Provided we have experimental data, we may determine approximations for unknown parameters, such as transport coefficients of diffusion, viscosity and thermal conductivity and use the resulting Euler equations or Navier-Stokes equations to describe the spatio-temporal evolution of the gas system. However, for a number of reasons, we do not have experimental data for all cases. Hence, a kinetic theoretical approach constitutes an important step in the understanding of a phenomenon and may be used to predict the result of an experiment, regarding specific values of the variables in consideration [17].

4 Linear Stability Analysis

In this section we will discuss the linear stability of the detonation wave solution obtained with the ZND model, which is an idealised model of the detonation problem. Moreover, linear stability analysis only allows us to evaluate the response of the detonation wave solution to small disturbances. Although this is a simplified problem, it reflects some of the important features of more realistic models and simultaneously allows an accurate mathematical approach.

As far as we know, the study of more complex and complete situations, such as multidimensional flows, is nearly non-existent. Furthermore, the difficulties of this approach already constitute an interesting mathematical challenge and, although some recent contributions and approaches to this problem have been made, there is still much to be done, namely in the efficiency of the numerical methods that are used to search for solutions.

The modern theory of detonation stability started with Erpenbeck, in 1962 [18, 19] and it is still the basis for the current stability work. Erpenbeck described the stability problem as an initial-value problem considering a small perturbation from the steady state. Along with other mathematical results, Erpenbeck used the Nyquist winding theorem to develop a numerical procedure that, for a given set of parameters, would determine the number of zeros of an analytic function in the complex plan. The zeros of this function corresponded to unstable solutions of the stability problem.

In 1990 Lee and Stewart [20] introduced a normal-mode approach and a numerical shooting method to develop a simpler and more efficient search for unstable solutions. After Erpenbeck's work, others, besides Lee and Stewart, contributed to the development of the stability analysis, namely [12, 13, 18, 21–23]. For more details on the state of detonation stability see [24].

In the next section, we present in more detail the procedure used to develop a linear stability analysis, using the normal-mode approach proposed in [20].

4.1 Stability Macroscopic Equations

It is well known from theoretical studies, as well as from experimental investigations, that steady solutions may degenerate into an oscillatory solution in the long-time limit. The first required test of the steady solutions should be the evaluation of its response to small rear boundary perturbations. To do that, we introduce a perturbation that induces a deviation on the shock wave position, giving rise to small perturbations on the state variables that propagate into the reaction zone. The evolution of the state variables perturbations over time determines the stability of the steady detonation solution. In fact, when some perturbation grows over time, the steady solution is said to be hydrodynamically unstable and if all perturbations decay in time, the steady solution is stable.

The linear stability problem is formulated as an initial-boundary value problem in terms of the stability differential equations, with initial conditions at the Von Neumann state and an additional closure boundary condition at the final state.

The equations for the study of the linear stability are obtained from the steady state equations attached to the shock front (16)–(19) and the initial Rankine–Hugoniot conditions (20)–(23). The shock front of a steady detonation wave with constant velocity D is placed in $x - Dt$ and if we introduce a perturbation on the shock front that depends on time we may write

$$x = x^{\ell} - \psi(t), \qquad \text{with} \qquad \psi(t) = Dt + \widetilde{\psi}(t), \tag{24}$$

where x^ℓ is the laboratory frame coordinate, $\widetilde{\psi}(t)$ the displacement of the shock wave from the unperturbed position due to a small perturbation, and $\psi(t)$ the location of the perturbed wave. In the new shock attached coordinate system, the instantaneous position of the perturbed shock wave is $x = 0$ and its velocity is $D(t) = D + \widetilde{\psi}'(t)$. Furthermore, a normal mode expansion with exponential time dependent perturbations is assumed for the steady state variables,

$$z(x,t) = z^*(x) + e^{at}\,\overline{z}(x), \qquad \psi(t) = \overline{\psi}\,e^{at}, \qquad a,\ \overline{\psi} \in \mathbb{C}, \tag{25}$$

where $z = [n_A\ n_B\ v\ p]^T$ is the state vector, $z^*(x)$ indicates the one-dimensional steady solution, $\overline{z}(x)$ is the vector of complex eigenfunctions representing the unknown spatially disturbances, $\overline{\psi}$ is a complex disturbance amplitude parameter and a is the complex eigenvalue, with Re a and Im a being the disturbance growth rate and frequency, respectively. The transformed governing equations in the perturbed shock frame are then linearized about the steady solution $z^*(x)$, by means of the expansions (25). Performing a further normalization of the state variables, with respect to the complex amplitude parameter $\overline{\psi}$, namely $\overline{w} = \overline{z}/\overline{\psi}$, one obtains the evolution equations in the wave coordinate x, for the complex disturbances. Rewriting $\overline{z}$ instead of $\overline{w}$, the resulting equations, for $x \in]x_F, 0[$, are

$$Da\overline{n}_\alpha + \left(v^* - D\right)\frac{d\overline{n}_\alpha}{dx} + \frac{n_\alpha^*}{dx}\left(\overline{v} - Da\right) + \frac{dv^*}{dx}\overline{n}_\alpha + n_\alpha^*\frac{d\overline{v}}{dx} = \overline{\tau}_\alpha, \qquad \alpha = A, B, \tag{26}$$

$$\rho^* Da\overline{v} + \frac{d\overline{p}}{dx} + \rho^*\frac{dv^*}{dx}\left(\overline{v} - Da\right) + \left(v^* - D\right)\frac{dv^*}{dx}\overline{\rho} + \rho^*\left(v^* - D\right)\frac{d\overline{v}}{dx} = 0, \tag{27}$$

$$Da\overline{p} + \frac{5}{3}\left(p^*\frac{d\overline{v}}{dx} + \overline{p}\frac{dv^*}{dx}\right) + \left(v^* - D\right)\frac{d\overline{p}}{dx} + \left(\overline{v} - Da\right)\frac{dp^*}{dx} = \frac{Q_R^* D\overline{\tau}_A}{3}, \tag{28}$$

with $\overline{\tau}_\alpha$ being the linearized reaction rates, explicitly presented in [16].

The initial conditions to be added to the stability Eqs. (26)–(28) are obtained by introducing the same expansion (25) and linearization about the steady solution as before, followed by a normalization with respect to $\overline{\psi}$. Hence, the resulting equations are:

$$\overline{n}_\alpha(0) = \frac{\left(n_\alpha^* - n_{\alpha 0}\right)a - n_\alpha^*\overline{v}(0)}{v^* - D}, \qquad \alpha = A, B, \tag{29}$$

$$\overline{v}(0) = \frac{3\rho_0 v^{*2} + \frac{3}{2}\left(p^* - p_0\right) - \frac{3}{2}D\rho_0 v^* + 2E_A n_0 + Q_R^* n_{B0}}{-\rho^*\left(v^* - D\right)^2 + \frac{5}{2}p^*}\,a\,, \tag{30}$$

$$\overline{p}(0) = -\rho_0 a v^* - \left(v^* - D\right)\rho^*\overline{v}(0)\,. \tag{31}$$

Equations (26)–(28) constitute the stability equations for the present modelling, giving the spatial evolution of the complex perturbations $\overline{z}(x)$ in the reaction zone, from the perturbed shock position $x = 0$, with initial conditions given by Eqs. (29)–(31), to the equilibrium final state $x = x_F$.

They form a system of eight first-order homogeneous linear ordinary differential equations with spatially varying coefficients, and eight initial conditions, for the real and imaginary parts of the complex perturbations and of the eigenvalue a. This system, which henceforward will be called stability system, is not closed and more information is needed to close it.

4.2 Radiation Condition

The radiation condition is called, in literature, the closure condition since it is used to close the stability equations system obtained in the previous subsection. This condition was adopted in many previous works on detonation stability as, for example, in papers [20, 24–28] and it is needed for physical purposes. This is a system of eight equations and ten variables therefore it is possible to consider two of those variables, for instance the real and the imaginary part of the eigenvalue a, as parameters and solve the system for the remaining eight variables. By doing so, we would obtain a solution for the stability system. However, this may not be a solution for the stability problem. In fact, the probability that the solution obtained in this manner could represent a solution for the stability problem is very low.

There are, in the above cited papers, some interesting explanations for the need to include this additional condition in order to obtain a physical solution to the problem. One argues that the detonation wave solution results exclusively from the interplay between the leading shock and the reaction zone and can not be affected by further disturbances traveling towards the shock from a great distance from the reaction zone. Regarding the adopted model, it has the expression:

$$\overline{v}(x_F) + a = \frac{-1}{\gamma \rho^*_{eq} c^*_{eq}} \, \overline{p}(x_F), \tag{32}$$

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

A solution of the linear stability problem of the steady detonation in terms of the complex disturbances $\overline{z}(x)$ and eigenvalue a must be obtained using the ordinary differential equations (26)–(28) for $x \in]x_F, 0[$, with initial conditions (29)–(31) at $x = 0$ and closure condition (32) at $x = x_F$. This problem was addressed in [16] as described in the next subsections.

4.3 Numerical Method

The stability problem is addressed numerically, with an iterative shooting technique based on the numerical method proposed by Lee and Stewart in paper [20], with the aim of obtaining the stability spectrum for the eigenfunction perturbations $\overline{z}$ and

eigenvalue perturbation parameter a, in terms of the parameters characterizing the steady solution. We choose a trial value of a in a fixed bounded domain $\mathscr{R}$ of the complex plane and then integrate Eqs. (26)–(28) in the reaction zone $]x_F, 0[$ with initial conditions (29)–(31) at $x = 0$, using a fourth order Runge–Kutta routine. The solution $\overline{z}(x)$, $x \in [x_F, 0]$, obtained for the considered trial value of a is then evaluated for $x = x_F$ to check if the boundary condition (32) is verified.

As was mentioned before, for a given steady detonation solution, an arbitrary value of a does not satisfy the closure condition (32) and thus the outcome is not a solution of the stability problem. To overcome this mishap, we may use the residual function $\mathscr{H}(a)$, defined from the closure condition (32) by the expression

$$\mathscr{H}(a) = \overline{v}(x_F) + a + \frac{1}{\gamma \rho^*_{eq} c^*_{eq}} \overline{p}(x_F), \quad a \in \mathbb{C}. \tag{33}$$

Notice that the radiation condition is verified if and only if $\mathscr{H}(a) = 0$, therefore to search for solutions considering the eigenvalue a to be in a limited region $\mathscr{R}$ of the complex plan, we may choose a large number of trial values a in that region and search for the zeros of $\mathscr{H}$. Although it looks like a simple task, the search for the zeros of $\mathscr{H}$ is a very time consumer task. There are some straightforward procedures introduced by Lee and Stewart in paper [20] but they require a huge number of trial values in a region of the complex plan, which implies that a regular computer needs a long period of time to do the calculations.

In paper [16] we introduced a numerical procedure to reduce the number of trial values that are needed to search for the zeros of $\mathscr{H}$. This procedure recovered the Erpenbeck's idea of counting the number of zeros of a function in a fixed domain of the complex plan and combined it with the shooting method proposed by Lee and Stewart. We believe that it is important to develop new and more efficient methods to search for zeros of the residual function, in order to help researchers in the development of a complete stability analysis on the detonation wave propagation. For more realistic cases, the calculations are even longer and those resources are all the more necessary.

In what follows, we present the numerical method that we used to count the number of zeros in a limited region of the complex plan.

Numerical Procedure

First we have to decide the region $\mathscr{R}$, of the complex plan, where we want to search for eigenvalues. With the expansion about the steady state defined in Eq. (25), we know that a stability solution is unstable if and only if $\mathrm{Re}\, a > 0$. We also know that it takes only one unstable solution to classify a steady detonation solution as unstable and that the existence of stable solutions bring no information about the stability of the steady detonation solution. Therefore, we must search for solutions in the right half of the complex plan. On the other hand, since these modes occur in conjugate pairs, it is enough to choose a domain $\mathscr{R}$ in the upper-right quarter of the complex plan.

The argument principle states that the difference between the number Z of zeros and P of poles of the function $\mathscr{H}$ within the region $\mathscr{R}$, provided that there are no

zeros in its contour, is given by

$$Z - P = \frac{1}{2\pi i} \int_{\zeta} \frac{\mathscr{H}'(u)}{\mathscr{H}(u)}\, du, \tag{34}$$

or equivalently by

$$Z - P = \frac{1}{2\pi i} \int_{k}^{\ell} \frac{\mathscr{H}'(\zeta(t))}{\mathscr{H}(\zeta(t))} \parallel \zeta'(t) \parallel dt, \tag{35}$$

where $\zeta : [k, \ell] \to \mathbb{C}$ is a path smooth by parts, describing the contour of $\mathscr{R}$ in the positive sense. We may consider that $\mathscr{H}$ does not have any poles, since we expect that the disturbancies do not blow in a finite time consistent with a linear analysis of the stability. Therefore we have $P = 0$ and the expression (35) gives the number of zeros of $\mathscr{H}$ inside the region $\mathscr{R}$,

$$Z = \frac{1}{2\pi i} \int_{k}^{\ell} \frac{\mathscr{H}'(\zeta(t))}{\mathscr{H}(\zeta(t))} \parallel \zeta'(t) \parallel dt. \tag{36}$$

The mean value theorem states that the integral in expression (36) is equal to the integral

$$\int_{k}^{\ell} \frac{\mathscr{H}'(\zeta(t))}{\mathscr{H}(\zeta(t))} \parallel \zeta'(t) \parallel dt = \mu(\ell - k), \tag{37}$$

where μ represents the mean value in the interval $[k, \ell]$ of the function h defined by

$$h(t) = \frac{\mathscr{H}'(\zeta(t))}{\mathscr{H}(\zeta(t))} \parallel \zeta'(t) \parallel, \quad t \in [k, \ell]\ . \tag{38}$$

Hence, to count the number of zeros in the region $\mathscr{R}$, all we need to compute is the value of μ.

It is well known that if n is large enough, then the mean value of the sample S, μ_S, can be treated as a statistical variable following a normal distribution with mean value μ and standard deviation $\sigma_S/\sqrt{n}$, where σ_S is the standard deviation of S. Therefore, the mean value μ of the function h can be inferred in a confidence interval by the mean value μ_S of the sample S. In this situation we considered

$$S = \left\{h(t_j) :\ i = 1, 2, \ldots, n\right\}, \tag{39}$$

with $t_j \in [k, \ell]$. To obtain the value of each $h(t_j)$, since we know path ζ, we directly obtain the values for $\zeta'(t_j)$ and $\zeta(t_j)$ and this last one is a point in the complex plan that might be used as a trial value to the eigenvalue a_j and thus solving the stability equation system, we obtain the value of $\mathscr{H}(\zeta(t_j))$. The value of $\mathscr{H}'(\zeta(t_j))$ is obtained choosing a suitable point close enough to $\zeta(t_j)$, say b_j, with $\mathrm{Re}\, b_j = \mathrm{Re}\, a_j + 10^{-6}$ and $\mathrm{Im}\, a_j = \mathrm{Im}\, b_j$, as follows

$$\mathscr{H}'(a_j) \approx \frac{\mathscr{H}(b_j) - \mathscr{H}(a_j)}{b_j - a_j}, \quad i = 1, 2, \ldots, n. \tag{40}$$

Consequently, the number of zeros of the residual function $\mathscr{H}$ inside the domain $\mathscr{R}$ is estimated as follows

$$\frac{\ell - k}{2\pi i}\left(\mu_S - 2.58\,\frac{\sigma_S}{\sqrt{n}}\right) < Z < \frac{\ell - k}{2\pi i}\left(\mu_S + 2.58\,\frac{\sigma_S}{\sqrt{n}}\right), \tag{41}$$

where the number 2.58 is used to assure the 99% confidence of the interval.

5 Discussion

The numerical procedure presented in the previous section requires a much smaller number of trial values than those needed to compute the methods presented by Lee and Stewart and is sufficient to determine if, given a specific set of parameters, a steady detonation is stable or not. This is precisely the information we have to have if we want to determine the stability boundary in some parameter plan such as the plan defined by the reaction heat and forward activation energy. On the other hand, if we want to determine the value of the eigenvalues, we need to proceed with the computation, considering subregions of $\mathscr{R}$ and using the numerical procedure considered above or applying the methods proposed by Lee and Stewart or even a combination of both.

We consider that it is important to improve this method or to create new ones to obtain solutions of the stability problem in order to increase the knowledge on the linear stability problem of the one-dimensional detonation wave as well as to approach more realistic models.

In paper [16] we were able to determine the region of the parameter plan of the reaction heat and forward activation energy that corresponds, giving a specific set of parameters, to unstable solution. Moreover, we tracked the fundamental eigenvalue along different values of the reaction heat. These are two examples of the nice perspectives that we might have on the macroscopic behaviour of a physical phenomenon such as a detonation wave, starting from the microscopic features of the system constituents and their relations.

Stability analysis is a major issue in the study of detonation waves which, in turn, are used to model many relevant engineering processes. As was said before, the model used in this paper is rather simplistic but still faces interesting challenges. We are already working on the development of a bidimensional stability analysis starting from a kinetic level and we expect to obtain new and interesting results on this subject.

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