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**Kinetic formulation of linear stability  
for steady detonation waves (\*\*)**

**1 - Introduction**

Aim of the present paper is to re-address the stability formulation of a detonation wave within a discrete kinetic framework, and, at the same time, show the capability of a kinetic model to study the linear stability, according to the classical treatment known in literature.

In a previous work [1], a mathematical procedure has been proposed in order to solve detonation problems by means of kinetic models for chemically reacting gases. Steady detonation waves in one-space dimension have been characterized for gases with a two-way reaction of bimolecular [1] or autocatalytic type [2]. Moreover, the sonic properties of the flow in thermodynamical equilibrium conditions have been studied, evaluating the frozen and equilibrium sound speeds [2]. The numerical values of steady wave solution have then been provided in paper [3], for the said chemical reactions.

It should be underlined that papers [1] and [2] have shown that the treatment of the detonation problem at a microscopic level, adopting the above mentioned kinetic models, provides many results which are in agreement with the ones of classical detonation theory, when they are transformed to the macroscopic scale, as

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pointed out in paper [3]. Furthermore, the microscopic analysis of the detonation wave problem allows a better description and detail of the chemical reactions which are fundamental to the detonation phenomenology.

As widely documented in experimental works, the detonation waves can induce non planar instabilities and turbulent reaction zones [4]. On the other hand, the detonation stability and the evolution of the instabilities are not easily described up to now; what concerns their exact and numerical treatment is essentially due to Erpenbeck [5], and later on to Lee & Stewart [6]. For all these reasons, it seems promising to deal with linear detonation stability from the point of view of discrete velocity models which exhibit a sufficiently simple mathematical structure [7], capable to perform the calculations discussed in the sequel.

In this paper, first of all, a class of discrete kinetic models for detonating gases with a quite general reversible chemical reaction is characterized, and the responses of the steady detonation solution to small rear boundary perturbations are then investigated at a microscopic scale.

Within such class of models, the stability equations are derived for detonation with a *finite length reaction zone*. At this end, a normal mode approach has been applied to the non linear reactive Euler equations of the model, according to the procedure outlined by Fickett [8], while the determinacy of the stability equations has been assured according to the analysis proposed by Lee & Stewart [6]. Their method for the calculation of linear detonation stability, which is simpler than the Erpenbeck's one [5] based on Laplace transforms, has here been adapted to the kinetic approach.

The contents of the present paper are arranged in six sections.

In section 2, the relevant mathematical aspects of a discrete model which can be adopted to describe the reactive flow are summarized, whereas the procedure necessary to recover detonation wave solutions is briefly outlined in section 3.

Starting from section 4, the stability problem is dealt with. In particular, the governing equations and related Rankine-Hugoniot conditions are transformed to the wave coordinate and then linearized through a normal mode expansion about the steady solution. After a further transformation to the steady reaction coordinate, the stability equations and suitable initial data are deduced in non closed form.

In section 5, an acoustic analysis is performed at the end of the reaction zone, and a radiation condition is imposed [6], in order to derive the dispersion relation of the normal modes. The stability equations with related initial data are then given in a closed form and their determinacy assured.

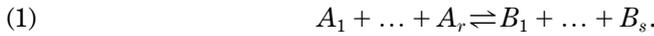
At last, in section 6, the stability problem is formulated for the general class of kinetic models of section 2, and a criterion for linear detonation stability is stated.

Concluding this section, it may be pertinent to underline that several mathematical aspects of the analysis carried on in this work are essentially based on the results obtained in a paper quoted [9].

## 2 - A class of discrete kinetic models for reacting gases

In this section, the main features of a class of discrete models for reacting gases are presented in a general form. Particular attention is devoted to the characterization of the collision invariant spaces and to both Maxwellian and thermodynamical equilibrium states, which are crucial to define the detonation wave solution.

Consider a gas mixture of  $r + s$  species  $A_1, \dots, A_r, B_1, \dots, B_s$ ,  $r, s \in \mathbb{N}$ , and let  $M$  denote the gas species, i.e.,  $M = A_1, \dots, A_r, B_1, \dots, B_s$ . Each gas species is identified by its molecular mass  $m_M$  and bond energy  $\varepsilon_M$ . Assume that the particles of each gas species  $M$  move in the space with velocities belonging to a prescribed finite set of  $p$  selected velocities  $\{v_i^M: i = 1, \dots, p\}$ ,  $v_i^M$  being the velocity of particles of  $M$ -species moving along the  $i$ -direction of the chosen geometry of the model. Elastic collisions preserve mass, momentum and kinetic energy, and result in a change of velocities only. Besides elastic collisions, the gas particles can interact according to the reversible chemical reaction



Inelastic collisions preserve mass, momentum and total energy (kinetic and bond), and result in a rearrangement of masses and energies.

Let  $N_i^M(\mathbf{x}, t)$ ,  $\mathbf{x} \in \mathbb{R}^3$ ,  $t \in \mathbb{R}_+$ , denote the distribution function of particles with velocity  $v_i^M$ . The microscopic state of the gas is given by the knowledge of the  $p(r + s)$  functions  $N_i^M$ , namely, the vector function  $N$ ,

$$N = (N_1^{A_1}, \dots, N_p^{A_1}, \dots, N_1^{A_r}, \dots, N_p^{A_r}, N_1^{B_1}, \dots, N_p^{B_1}, \dots, N_1^{B_s}, \dots, N_p^{B_s}).$$

In order to study one-dimensional detonation stability, the kinetic equations and the governing equations of the model will be written in one space dimension. The distribution functions will then be denoted by  $N_i^M(x, t)$ ,  $x \in \mathbb{R}$ ,  $t \in \mathbb{R}_+$ .

### Kinetic equations

It is known that the time-space evolution of  $N_i^M(x, t)$  result from *gains* and *losses* of particles with velocity  $v_i^M$  during elastic scattering and from *sources* and *sinks* due to inelastic interactions. The behaviour of the functions  $N_i^M$  is specified by the *kinetic equations* of the model, which constitute an hyperbolic set of semi-

linear partial differential equations of type

$$(2) \quad \left( \frac{\partial}{\partial t} + v_i^M \frac{\partial}{\partial x} \right) N_i^M = Q_i^M(\mathbf{N}) + \mathcal{R}_i^M(\mathbf{N}).$$

In Eq. (2),  $v_i^M$  is the component of  $\mathbf{v}_i^M$  along the  $x$ -direction, and  $Q_i^M(\mathbf{N})$ ,  $\mathcal{R}_i^M(\mathbf{N})$  represent the nonlinear one-dimensional collision terms associated to elastic scattering and inelastic interactions, respectively. The analytical form of  $Q_i^M(\mathbf{N})$  and  $\mathcal{R}_i^M(\mathbf{N})$  depends on the geometry of the chosen model, whereas their definition through the balance between gain and loss terms, as well as source and sink terms, is already known in the literature (see [7], [9]). With the vector functions

$$\mathbf{Q} = \{ Q_i^M \}_{i=1, \dots, p}^{M=A_1, \dots, A_r, B_1, \dots, B_s},$$

$$\mathbf{R} = \{ \mathcal{R}_i^M \}_{i=1, \dots, p}^{M=A_1, \dots, A_r, B_1, \dots, B_s},$$

the kinetic equations (2) can be written in matrix form

$$(3) \quad \frac{\partial \mathbf{N}}{\partial t} + \mathcal{C} \mathbf{N} = \mathbf{Q}(\mathbf{N}) + \mathbf{R}(\mathbf{N}),$$

where  $\mathcal{C}$  is a square matrix of order  $p(r+s)$  with non-zero elements  $\mathcal{C}_{ii} = v_i^M \frac{\partial}{\partial x}$ .

### Macroscopic variables

In discrete kinetic theory, the macroscopic description of the gas is achieved by definition of suitable mean quantities [7]. For the models here considered, such quantities can be expressed by

$$(4) \quad \langle \mathbf{Y}, \mathbf{N} \rangle = \sum_M \sum_{i=1}^p Y_i^M N_i^M,$$

where  $\mathbf{Y}$ , defined by

$$\mathbf{Y} = (Y_1^{A_1}, \dots, Y_p^{A_1}, \dots, Y_1^{A_r}, \dots, Y_p^{A_r}, Y_1^{B_1}, \dots, Y_p^{B_1}, \dots, Y_1^{B_s}, \dots, Y_p^{B_s}),$$

is a vector function whose  $p(r+s)$  components depend on the selected velocities, and  $\langle \cdot, \cdot \rangle$  represents the inner product in  $\mathbb{R}^{p(r+s)}$ .

In particular, the mass density of  $M$ -species  $\rho_M$ , total mass density  $\rho$ , momen-

tum  $Q$  along the  $x$ -direction, kinetic energy  $T$  and total energy  $E$  have the form

$$(5) \quad \begin{aligned} \varrho_M &= m_M \sum_{i=1}^p N_i^M, & \varrho &= \sum_M \varrho_M, \\ Q &= \sum_M m_M \sum_{i=1}^p N_i^M v_i^M, \\ T &= \sum_M \sum_{i=1}^p \frac{1}{2} m_M |\mathbf{v}_i^M|^2 N_i^M, \\ E &= \sum_M \sum_{i=1}^p \left( \frac{1}{2} m_M |\mathbf{v}_i^M|^2 + \varepsilon_M \right) N_i^M, \end{aligned}$$

as it turns out from definition (4), when one of the following five expressions for  $Y$  is considered, respectively:

$$(i) \quad Y = \{Y_i^{M'}\}_{i=1, \dots, p}^{M'=A_1, \dots, A_r, B_1, \dots, B_s},$$

where  $Y_i^{M'} = m_M$  if  $M' = M$  and  $Y_i^{M'} = 0$  if  $M' \neq M$ ,  $i = 1, \dots, p$ ;

$$(ii) \quad Y = \{Y_i^M\}_{i=1, \dots, p}^{M=A_1, \dots, A_r, B_1, \dots, B_s},$$

where  $Y_i^M = m_M$ ,  $i = 1, \dots, p$ ;

$$(iii) \quad Y = \{m_M v_i^M\}_{i=1, \dots, p}^{M=A_1, \dots, A_r, B_1, \dots, B_s};$$

$$(iv) \quad Y = \left\{ \frac{1}{2} m_M |\mathbf{v}_i^M|^2 \right\}_{i=1, \dots, p}^{M=A_1, \dots, A_r, B_1, \dots, B_s};$$

$$(v) \quad Y = \left\{ \frac{1}{2} m_M |\mathbf{v}_i^M|^2 + \varepsilon_M \right\}_{i=1, \dots, p}^{M=A_1, \dots, A_r, B_1, \dots, B_s}.$$

### Rate equation

The chemical composition of the gas is specified by the *progress variable* of the model,  $\lambda$ , defined as the number density of a given gas species, which results to be a product of the forward reaction. Without loss of generality,  $\lambda$  is here given by the number density of  $B_1$ -species, that is

$$(6) \quad \lambda(x, t) = \sum_{i=1}^p N_i^{B_1}(x, t), \quad x \in \mathbb{R}, \quad t \geq 0,$$

or, equivalently, in macroscopic form,

$$(7) \quad \lambda(x, t) = \frac{\varrho_{B_1}}{m_{B_1}}(x, t),$$

where  $\varrho_{B_1} = m_{B_1} \sum_{i=1}^p N_i^{B_1}$  is the mass density of  $B_1$ .

According to its meaning, the progress variable  $\lambda$  increases from 0, when the  $B_1$ -species is absent, to the value  $\lambda_e$  when the reaction reaches the chemical equilibrium. The behaviour of  $\lambda$  is justified by the fact that the gas tends towards the chemical equilibrium in a non reversible way. Such gas evolution is assured by the existence of an  $\mathcal{H}$ - functional which exhibits a monotone non increasing behaviour in time.

If one takes into account definition (6) of  $\lambda$  and kinetic equations (2) for the  $B_1$ -species, the time-space evolution of  $\lambda$  is described by

$$(8) \quad \frac{d\lambda}{dt} = \sum_{i=1}^p (Q_i^{B_1}(\mathbf{N}) + \mathcal{R}_i^{B_1}(\mathbf{N})),$$

where  $d/dt$  is the Lagrangian derivative. Equation (8) is the rate equation of the model.

Due to the explicit expressions of the collision terms  $Q_i^M(\mathbf{N})$  and  $\mathcal{R}(\mathbf{N})_i^M$ , Eq. (8) can be rearranged in the usual form in chemical kinetics [9], that is

$$(9) \quad \frac{d\lambda}{dt} = r_f - r_b,$$

where  $r_f = r_f(\varrho_{A_1}, \dots, \varrho_{A_r}; \nu_f)$ ,  $r_b = r_b(m_{B_1}\lambda, \varrho_{B_2}, \dots, \varrho_{B_s}; \nu_b)$  denote the forward and backward reaction rates depending on the mass densities of the related reactants, and on constant reactive collision frequencies  $\nu_f, \nu_b$ . The vanishing of the right hand-side of Eq. (9) determines the chemical equilibrium condition of the model

$$r_f(\varrho_{A_1}, \dots, \varrho_{A_r}; \nu_f) = r_b(m_{B_1}\lambda, \varrho_{B_2}, \dots, \varrho_{B_s}; \nu_b)$$

corresponding to equal rates of production of species  $A_1, \dots, A_r$  and  $B_1, \dots, B_s$ . Its microscopic formulation, recalling expression (5) of  $\varrho_M$ , is

$$(10) \quad r_f(N_1^{A_1}, \dots, N_p^{A_r}; \nu_f) = r_b(N_1^{B_1}, \dots, N_p^{B_s}; \nu_b).$$

### Collision invariants

According to the theory developed in [9], two types of collision invariants can

be defined for the class of models previously introduced: the *mechanical* collision invariants associated to elastic scattering only, necessary to define the Maxwellian equilibrium state, and the *mechanical-reactive* collision invariants associated to both elastic and inelastic collisions, necessary to deduce the conservation equations of the model. For sake of clarity, some preliminaries will be recalled.

Definition 1.  $Y$  is a *mechanical collision invariant* iff

$$(11) \quad \langle Y, \mathbf{Q}(N) \rangle = 0 .$$

The set of all mechanical collision invariants is denoted by  $\mathcal{F}$ . ■

Definition 2.  $Y$  is a *mechanical-reactive collision invariant* iff

$$(12) \quad \langle Y, \mathbf{Q}(N) \rangle = 0 , \quad \langle Y, \mathbf{R}(N) \rangle = 0 .$$

The set of all mechanical-reactive collision invariants is denoted by  $\mathcal{M}$ . ■

For each  $Y \in \mathcal{F}$ , the corresponding macroscopic variable  $\langle Y, N \rangle$  is preserved during elastic collisions, whereas for each  $Y \in \mathcal{M}$ , the corresponding macroscopic variable  $\langle Y, N \rangle$  is preserved during both elastic collisions and chemical interactions. Therefore, the elements  $Y \in \mathcal{M}$  determine the conservation equations of the model.

On the other hand, the elements  $Y \in \mathcal{F}$  define the Maxwellian state of mechanical equilibrium, as it will be clear when the thermodynamical equilibrium state will be dealt with.

Proposition 1. *The sets  $\mathcal{F}$  and  $\mathcal{M}$  are linear subspaces of  $\mathbb{R}^{p(r+s)}$  with  $\mathcal{M} \subset \mathcal{F}$ . The dimensions  $q$  of  $\mathcal{F}$  and  $q_{\mathcal{R}}$  of  $\mathcal{M}$  are such that*

$$1 \leq q_{\mathcal{R}} < q \leq p(r+s),$$

and

$$q_{\mathcal{R}} = q - 1 . \quad \blacksquare$$

This proposition is proven in paper [9].

*Basis of  $\mathcal{M}$  and  $\mathcal{F}$*

Let the set  $\mathcal{B}_{\mathcal{M}}$ ,

$$\mathcal{B}_{\mathcal{M}} = \{ Y^{(1)}, \dots, Y^{(q-1)} \},$$

denote a basis of  $\mathfrak{M}$  and  $Y^{(q)}$  be a vector function in  $\mathcal{F}$  which is not in  $\mathfrak{M}$ . Thanks to Proposition 1, it is possible to consider the set  $\mathcal{B}_{\mathcal{F}}$ ,

$$(13) \quad \mathcal{B}_{\mathcal{F}} = \{Y^{(1)}, \dots, Y^{(q-1)}, Y^{(q)}\}, \quad \mathcal{B}_{\mathfrak{M}} \subset \mathcal{B}_{\mathcal{F}},$$

as a basis of  $\mathcal{F}$ .

According to definition (4),  $Y^{(q)}$  determines a macroscopic variable which is preserved during elastic collisions only. In particular, one can choose

$$(14) \quad Y^{(q)} = \{[Y^{(q)}]_i^M\}_{i=1, \dots, p}^{M=A_1, \dots, A_r, B_1, \dots, B_s},$$

where  $[Y^{(q)}]_i^{B_1} = 1$  and  $[Y^{(q)}]_i^M = 0$  for  $M \neq B_1$ . The corresponding macroscopic variable is

$$\langle Y^{(q)}, \mathbf{N} \rangle = \sum_{i=1}^p N_i^{B_1},$$

which identifies the progress variable  $\lambda$  introduced in Eq. (6).

### Conservation equations

The following equations

$$(15) \quad \left\langle \frac{\partial \mathbf{N}}{\partial t}, Y^{(k)} \right\rangle + \langle \mathcal{C} \mathbf{N}, Y^{(k)} \rangle = 0, \quad Y^{(k)} \in \mathcal{B}_{\mathfrak{M}}, \quad k = 1, \dots, q-1,$$

constitute a set of independent conservation equations, obtained from Eq. (3) and conditions (12). Each of them corresponds to the conservation of the macroscopic variable  $\langle \mathbf{N}, Y^{(k)} \rangle$  as, in particular, total mass density, momentum, and total energy.

The macroscopic evolution of the gas is characterized by means of the conservation equations (15) plus the rate equation (9), which can be rewritten as

$$(16) \quad \left\langle \frac{\partial \mathbf{N}}{\partial t}, Y^{(q)} \right\rangle + \langle \mathcal{C} \mathbf{N}, Y^{(q)} \rangle = r_f(N_1^{A_1}, \dots, N_p^{A_r}; \nu_f) - r_b(N_1^{B_1}, \dots, N_p^{B_s}; \nu_b).$$

The  $q$  equations (15), (16) do not form, in general, a closed set, since  $p(r+s)$  unknown distribution functions  $N_i^M$  are involved. However, such a set becomes closed when the unknowns are referred to a particular state of the gas, the Maxwellian state, characterized by  $q$  parameters only, as it will be clarified below.

### Thermodynamical equilibrium

The complete thermodynamical equilibrium state of a reacting gas implies bo-

th mechanical and chemical equilibrium. The mechanical equilibrium is reached much faster than the chemical one because the relaxation time of elastic interactions is small when compared with the relaxation time of the chemical reaction [10]. For this reason, the mechanical equilibrium is regarded as a form of partial equilibrium, called Maxwellian, from which the gas can only evolve to a state of complete thermodynamical equilibrium.

The Maxwellian and thermodynamical equilibrium states of the gas are characterized through the  $\mathcal{H}$ -theorem which provides microscopic conditions for the distribution functions  $\widehat{N}_i^M$  of Maxwellian equilibrium and  $\widetilde{N}_i^M$  of thermodynamical equilibrium, as defined below.

The  $\mathcal{H}$ -theorem, related to a gas mixture undergoing chemical reversible reaction of type (1), has been formulated and proven in Ref. [9].

### Maxwellian state

Introduce the vector function  $\log \mathbf{N} \in \mathbb{R}^{p(r+s)}$ , given by

$$\log \mathbf{N} = (\log N_1^{A_1}, \dots, \log N_p^{A_r}, \log N_1^{B_1}, \dots, \log N_p^{B_s}).$$

The Maxwellian state is such that

$$(17) \quad \mathbf{N} = \widehat{\mathbf{N}} \quad \text{iff} \quad \log \mathbf{N} \in \mathcal{F},$$

or, equivalently,

$$N_i^M = \widehat{N}_i^M \quad \text{iff} \quad \log N_i^M = \sum_{j=1}^q d_j [Y^{(j)}]_i^M, \quad i = 1, \dots, p,$$

since  $\mathcal{F}$  is spanned by  $\mathcal{B}_{\mathcal{F}}$  (see Eq. (13)). Coefficients  $d_j = d_j(x, t)$ ,  $j = 1, \dots, q$ , are the so called Maxwellian parameters of the model and  $[Y^{(j)}]_i^M$ ,  $i = 1, \dots, p$ ,  $M = A_1, \dots, A_r, B_1, \dots, B_s$ , are the components of  $Y^{(j)}$ .

Hence, the Maxwellian state of the gas is characterized by

$$(18) \quad \widehat{N}_i^M = \exp \left( \sum_{j=1}^q d_j [Y^{(j)}]_i^M \right).$$

All macroscopic variables of such state can then be determined in terms of the Maxwellian parameters. For mathematical convenience,  $d_1, \dots, d_q$  are replaced by  $z_1 = \exp d_1, \dots, z_q = \exp d_q$ . In the sequel,  $z_1(x, t), \dots, z_q(x, t)$  will be referred to as the *Maxwellian parameters of the model*. Moreover,  $z_q$  is conventionally set

equal to zero when  $B_1$ -species is absent. Expressions (18) become

$$(18a) \quad \widehat{N}_i^M = \prod_{j=1}^q (z_j)^{[r^{(j)}]_i^M},$$

and, in particular, the *progress variable*  $\lambda$  in the *Maxwellian state* is given by

$$(19) \quad \lambda = \sum_{i=1}^p \prod_{j=1}^q (z_j)^{[r^{(j)}]_i^{B_1}}.$$

Inserting expressions (14) into Eq. (19), one gets

$$(20) \quad \lambda = z_q \sum_{i=1}^p \prod_{j=1}^{q-1} (z_j)^{[r^{(j)}]_i^{B_1}}.$$

Observe that the vanishing of the progress variable  $\lambda$  implies  $z_q = 0$ .

### *Thermodynamical equilibrium state*

A state of complete thermodynamical equilibrium is such that

$$N = \widetilde{N} \quad \text{iff} \quad \log N \in \mathfrak{N},$$

or, equivalently,

$$(21) \quad N_i^M = \widetilde{N}_i^M \quad \text{iff} \quad N_i^M = \widehat{N}_i^M \quad \text{and} \quad r_f(\widehat{N}_1^{A_1}, \dots, \widehat{N}_p^{A_p}; \nu_f) = r_b(\widehat{N}_1^{B_1}, \dots, \widehat{N}_p^{B_s}; \nu_b).$$

In terms of the Maxwellian parameters, taking into account expressions (18a), the microscopic chemical equilibrium condition can be rewritten as

$$(22) \quad r_f(z_1, \dots, z_q; \nu_f) = r_b(z_1, \dots, z_q; \nu_b).$$

### **Reactive Euler equations**

The reactive Euler equations of the model are the  $q - 1$  conservation equations (15) plus the rate equation (16), referred to the Maxwellian state. Accordingly, insert expressions (18a), (20) into Eqs. (15), (16), and rearrange the time and space derivatives in terms of the Maxwellian parameters  $z_1, \dots, z_q$ . The resulting equations, referred to the laboratory frame  $(x^l, t)$  assume the matrix form

$$(23) \quad B(\mathbf{z}) \frac{\partial \mathbf{z}}{\partial t} + A(\mathbf{z}) \frac{\partial \mathbf{z}}{\partial x^l} = \mathbf{c}(\mathbf{z}),$$

where  $\mathbf{z} = [z_1 \dots z_q]^T$  denotes the state vector of the model,  $\mathbf{z} = \mathbf{z}(x^l, t)$ , the  $q$ -square matrices  $B$  and  $A$  are known first order homogenous functions of  $\mathbf{z}$ , since the model has been reduced to one-space dimension, as already said at the beginning of the present section, and the vector  $\mathbf{c}$  has components

$$c_1 = \dots = c_{q-1} = 0, \quad c_q = r_f(z_1, \dots, z_q; \nu_f) - r_b(z_1, \dots, z_q; \nu_b).$$

The explicit form of  $B$ ,  $A$  and  $\mathbf{c}$  depends on the chosen kinetic model. Note that system (23) results to be hyperbolic, as it has been proven in Ref. [9].

### 3 - Detonation wave solutions

The one-dimensional steady detonation with a two-way chemical reaction is well described by the so called ZND model, due to Zeldovich, von Neumann and Doering, extended to reversible reactions (see Ref. [8]). The structure of the detonation wave is represented in Fig. 1: the lead element is a non-reactive shock wave propagating with constant velocity, followed by a finite reaction zone, connecting the von Neumann state  $N$  to the final equilibrium state  $S$ ; all intermediate states of partial reaction are represented by  $R$ , and the initial state, ahead of the wave, by  $I$ ;  $x_B$  refers to the rear boundary,  $x_S$ ,  $x_R$  and  $x_0$  to the final, intermediate and initial states, respectively, and  $\mathcal{O}$  is the constant shock wave velocity. A discrete kinetic approach to the steady detonation problem, based on ZND description, may be realized within the class of discrete models proposed in section 2.

The governing equations of the reactive flow, referred to the laboratory frame, are given by the matrix equation (23). In order to get the steady detonation solutions, Eq. (23) is first transformed to the steady frame attached to the shock wave.

Introduce the transformation  $x^* = x^l - \mathcal{O}^l t$ ,  $\tau = t$  so that

$$\frac{\partial}{\partial t} = -\mathcal{O}^l \frac{\partial}{\partial x^*} + \frac{\partial}{\partial \tau}, \quad \frac{\partial}{\partial x^l} = \frac{\partial}{\partial x^*}.$$

Recalling that in the steady frame  $\frac{\partial}{\partial \tau} = 0$  and the partial derivative with respect to  $x^l$  becomes ordinary with respect to  $x^*$ , the (q-1) conservation equations, coming from Eq. (23), assume the form

$$(24) \quad [\mathcal{O}^l K(\mathbf{z}) + L(\mathbf{z})] \frac{d\mathbf{z}}{dx^*} = 0.$$

In Eq. (24) the state vector is now  $\mathbf{z} = \mathbf{z}(x^*)$ ,  $K(\mathbf{z})$  and  $L(\mathbf{z})$  are  $(q-1) \times q$  matrices.

ces obtained from  $-B(\mathbf{z})$  and  $A(\mathbf{z})$ , respectively, extracting the first  $(q - 1)$  rows. Thus the matrices  $K$  and  $L$  are also first order homogenous functions of  $\mathbf{z}$ .

Across the shock wave, the unknown  $\mathbf{z}$  is related by the  $q - 1$  Rankine-Hugoniot conditions which express the conservation of suitable macroscopic quantities between the states immediately ahead and behind the shock. These jump conditions are deduced from the conservation equations (24), by integration between the initial state  $I$ , ahead of the wave, and an arbitrary von Neumann state  $N$ , intermediate state  $R$ , or final state  $S$ , behind. Their matrix form, with the detonation velocity  $\mathcal{O}^l$  as parameter, is

$$(25) \quad [\mathcal{O}^l K(\mathbf{z}) + L(\mathbf{z})] \mathbf{z} = \mathcal{O}^l \mathbf{w}_0,$$

where  $\mathbf{w}_0$  is a  $(q - 1)$ -component vector depending on the  $\mathbf{z}$ -value,  $\mathbf{z}_0$ , at the initial state  $I$  and detonation velocity  $\mathcal{O}^l$ , i. e.

$$\mathbf{w}_0 = K(\mathbf{z}_0) \mathbf{z}_0 + \frac{1}{\mathcal{O}^l} L(\mathbf{z}_0) \mathbf{z}_0.$$

The Rankine-Hugoniot conditions (25) are fundamental to the description of the steady detonation solution, once a pertinent model of section 2 has been selected. In fact, the knowledge of the microscopic steady solution of Eq. (25), say  $\mathbf{z}^*$ , implies that all states  $N$ ,  $R$ ,  $S$  can be computed for every admissible detonation velocity  $\mathcal{O}^l$ . The Hugoniot diagram can then be plotted, exhibiting different Rayleigh lines through the initial state  $I$ , and different detonation Hugoniot curves of no reaction, partial reaction and equilibrium states.

The following flow can then be characterized, for assigned rear boundary condition, and the wave thickness computed, as well, for assigned initial condition at the von Neumann state.

In particular, the structure of the steady detonation wave solutions has been determined for bimolecular [2] and autocatalytic [3] reactions, as already mentioned in the introduction.

#### 4 - Linear detonation stability problem

The detonation stability is classically studied assuming that a small rear boundary perturbation, instantaneously assigned, induces a distortion on the steady planar shock wave, whereas subsequent rear oscillations do not affect the shock wave [6]. The reactive Euler equations (23) and related shock conditions (25) are linearized through a normal mode expansion about the steady detonation solution. The linearized equations define the evolution of the responses of the system to the

above mentioned perturbations. The resulting stability problem is formulated in the wave coordinate and afterwards in the more convenient steady reaction coordinate.

#### 4.1 - Formulation in the wave coordinate

The state variables will be first referred to the *wave coordinate*, which measures the distance from the perturbed shock. Let  $\psi(t)$  denote the position of the perturbed shock wave,

$$(26) \quad \psi(t) = \mathcal{O}^l t + \psi^l(t),$$

where  $\mathcal{O}^l$  is the constant velocity of the unperturbed shock relative to the laboratory frame, and  $\psi^l(t)$  the distortion on the position of the shock wave. The perturbed shock velocity is then

$$(27) \quad \mathcal{O}(t) = \mathcal{O}^l + \frac{d\psi^l}{dt}(t).$$

Let  $x$  denote the wave coordinate in the frame attached to the perturbed shock wave; the new coordinates are

$$(28) \quad x = x^l - \psi(t), \quad t = t,$$

and the space and time derivatives become  $\partial/\partial x$  and  $\partial/\partial t - (\mathcal{O}^l + d\psi^l/dt) \partial/\partial x$ , respectively. Therefore, Eqs. (23), (25) transform to

$$(29) \quad B(\mathbf{z}) \frac{\partial \mathbf{z}}{\partial t} + \left[ A(\mathbf{z}) - \left( \mathcal{O}^l + \frac{d\psi^l}{dt} \right) B(\mathbf{z}) \right] \frac{\partial \mathbf{z}}{\partial x} = \mathbf{c}(\mathbf{z}),$$

and

$$(30) \quad \left[ \left( \mathcal{O}^l + \frac{d\psi^l}{dt}(t) \right) K(\mathbf{z}) + L(\mathbf{z}) \right] \mathbf{z} = \left( \mathcal{O}^l + \frac{d\psi^l}{dt}(t) \right) \mathbf{w}_0,$$

where  $B, A, \mathbf{c}, K, L$  are here written in the wave coordinate (28).

Equations (29)-(30) will be now linearized through a normal mode expansion about the known steady solution  $\mathbf{z}^*(x)$ . According to paper [11], assume that all perturbations of the state vector components have an exponential time dependence, so that approximate solutions are sought in the form

$$(31) \quad \mathbf{z}(x, t) = \mathbf{z}^*(x) + \exp(at) \bar{\mathbf{z}}(x), \quad \psi^l(t) = \bar{\psi} \exp(at), \quad a, \bar{\psi} \in \mathbb{C} - \{0\},$$

where the sign of the real part of  $a$  determines the stability behaviour of the steady solution.

Hereinafter the starred quantities denote the steady character of the known solution, while the bar refers to the disturbance. From expansions (31) it follows

$$(32) \quad \begin{aligned} \frac{\partial \mathbf{z}}{\partial t} &= a \exp(at) \bar{\mathbf{z}} \\ \frac{\partial \mathbf{z}}{\partial x} &= \frac{d\mathbf{z}^*}{dx} + \exp(at) \frac{d\bar{\mathbf{z}}}{dx} \\ \frac{d\psi^l}{dt} &= a\bar{\psi} \exp(at), \end{aligned}$$

where  $\frac{d\mathbf{z}^*}{dx}$  is a known steady vector function. Taking into account the normal modes (31) and neglecting the nonlinear terms with respect to  $\bar{\mathbf{z}}$ , the coefficient matrices  $B$ ,  $A$ ,  $\mathbf{c}$ ,  $K$ ,  $L$  of Eqs. (29)-(30) can be expanded in the form

$$(33) \quad \begin{aligned} B(\mathbf{z}) &= B^*(\mathbf{z}^*) + \exp(at) B_1(\mathbf{z}^*) \bar{\mathbf{z}} \mathbf{r}^T \\ A(\mathbf{z}) &= A^*(\mathbf{z}^*) + \exp(at) A_1(\mathbf{z}^*) \bar{\mathbf{z}} \mathbf{r}^T \\ \mathbf{c}(\mathbf{z}) &= \mathbf{c}^*(\mathbf{z}^*) + \exp(at) C_1(\mathbf{z}^*) \bar{\mathbf{z}} \end{aligned}$$

$$(34) \quad \begin{aligned} K(\mathbf{z}) &= K^*(\mathbf{z}^*) + \exp(at) K_1(\mathbf{z}^*) \bar{\mathbf{z}} \mathbf{r}^T \\ L(\mathbf{z}) &= L^*(\mathbf{z}^*) + \exp(at) L_1(\mathbf{z}^*) \bar{\mathbf{z}} \mathbf{r}^T, \end{aligned}$$

where the starred matrices simply denote the corresponding ones evaluated in the steady state,  $B_1$ ,  $A_1$ ,  $C_1$ ,  $K_1$ ,  $L_1$  are again constant matrices resulting from the linearization process and  $\mathbf{r}^T$  is a constant  $q$ -row vector suitable to adjust the dimension of the perturbation terms in the above matrix expansions. Note that  $\mathbf{r}^T$  depends on the chosen model.

Moreover, in expressions (33)  $B_1$ ,  $A_1$  and  $C_1$  are  $q$ -square matrices, whereas in expressions (34)  $K_1$  and  $L_1$  are  $(q-1) \times q$  matrices.

#### Linear stability equations in the wave coordinate

Inserting expansions (31)-(33) in Eqs. (29), the linearized Euler equations are deduced as

$$(35) \quad (A^* - \mathcal{O}^l B^*) \frac{d\bar{\mathbf{z}}}{dx} + \left[ \mathbf{r}^T \frac{d\mathbf{z}^*}{dx} (A_1 - \mathcal{O}^l B_1) + aB^* - C_1 \right] \bar{\mathbf{z}} - a\bar{\psi} B^* \frac{d\mathbf{z}^*}{dx} = 0.$$

Equations (35), which give the space evolution of the disturbances  $\bar{z}(x)$  behind the shock, are the linear stability equations in the wave coordinate.

#### Initial conditions in the wave coordinate

Inserting expansions (31), (34) in Eqs. (30), the linearized Rankine-Hugoniot conditions are deduced in the form

$$(36) \quad [\mathcal{O}^l K^* + L^* + \mathbf{r}^T \mathbf{z}^* (\mathcal{O}^l K_1 + L_1)] \bar{z} = a \bar{\psi} (-K^* \mathbf{z}^* + \mathbf{w}_0).$$

The perturbed Rankine-Hugoniot conditions (36) relate the value of the disturbances  $\bar{z}$  in the reaction zone to their zero value at the initial state. These jump relations, when specifically referred to the von Neumann state, namely

$$\mathbf{z}_{VN}(t) = \mathbf{z}_{VN}^* + \exp(at) \bar{z}_{VN},$$

provide  $q - 1$  initial conditions for the  $q$  differential equations (35), i.e.

$$(36a) \quad [\mathcal{O}^l K_{VN}^* + L_{VN}^* + \mathbf{r}^T \mathbf{z}_{VN}^* (\mathcal{O}^l K_1 + L_1)_{VN}] \bar{z}_{VN} = a \bar{\psi} (-K_{VN}^* \mathbf{z}_{VN}^* + \mathbf{w}_0).$$

The further initial condition to be joined to Eq. (35), as justified in Remark 1, results to be

$$(36b) \quad (\bar{z}_q)_{VN} = 0.$$

Thus, the  $q$  initial conditions (36a, b) at the von Neumann state can be rewritten in compact form

$$(37) \quad P \bar{z}_{VN} = a \bar{\psi} \mathbf{h},$$

with  $P = P(\mathbf{z}_{VN}^*)$  a  $q$ -square matrix and  $\mathbf{h} = \mathbf{h}(\mathbf{z}_{VN}^*, \mathbf{w}_0)$  a  $q$ -component vector, as detailed in Remark 2.

In conclusion, the linear stability problem is formulated, in the wave coordinate, in terms of the complex disturbance  $\bar{z}$  and growth rate  $a$ , by means of the initial value problem (35), (37).

On the other hand, it is convenient to transform such a problem to the steady reaction coordinate, since the steady states in the reaction zone are characterized for each value of the progress variable  $\lambda$ . This is the object of the next subsection.

Remark 1. Remember that at the von Neumann state the chemical reaction has not yet started so that the progress variable  $\lambda$  there is still zero

$$\lambda(\mathbf{z}_{VN}) = 0.$$

Therefore expression (20), referred to the von Neumann state, gives

$$(z_q)_{VN} = 0,$$

and, in terms of the normal mode expansion (31),

$$(z_q^*)_{VN} + \exp(at)(\bar{z}_q)_{VN} = 0.$$

Since  $(z_q^*)_{VN} = 0$ , Eq. (36b) immediatly follows. ■

**Remark 2.** In Eq. (37),  $P$  is formed by the  $(q-1) \times q$  matrix  $[\mathcal{O}^l K_{VN}^* + L_{VN}^* + \mathbf{r}^T \mathbf{z}_{VN}^* (\mathcal{O}^l K_1 + L_1)_{VN}]$  augmented by the row  $[0 \dots 01]$ , while  $\mathbf{h}$  is formed by the  $(q-1)$ -component vector  $-K_{VN}^* \mathbf{z}_{VN}^* + \mathbf{w}_0$  augmented by the element 0. ■

#### 4.2 - Formulation in the steady reaction coordinate

For a single chemical reaction of type (1), the progress variable  $\lambda \in [0, \lambda_e]$  is monotonically increasing with respect to the distance from the shock front in the reaction zone. For this reason, it is possible to avoid the explicit  $x$ -dependence, replacing the wave coordinate  $x$  by the *steady reaction coordinate*  $s$ ,

$$(38) \quad s = \lambda^*(x), \quad s \in [0, \lambda_e^*].$$

The space derivative becomes

$$(39) \quad \frac{d}{dx} = \frac{r^*}{v_{B_1}^*} \frac{d}{ds},$$

where  $v_{B_1}^*$  is the velocity of  $B_1$ -particles and  $r^* = r_f^*(z_1, \dots, z_q; \nu_f) - r_b^*(z_1, \dots, z_q; \nu_b)$  the reaction rate referred to the steady state. For mathematical convenience, the perturbation  $\bar{z}$  will be normalized with respect to its value at the von Neumann state.

#### Normalization

Let  $\mathbf{d}$  denote the  $q$ -component vector

$$\mathbf{d} = [1 \dots 10]^T,$$

and  $S = S(\bar{z}_{VN})$  the  $q$ -diagonal matrix

$$S = \begin{bmatrix} S_{11} & 0 & 0 & \dots & 0 & 0 \\ 0 & S_{22} & 0 & \dots & 0 & 0 \\ 0 & 0 & S_{33} & \dots & 0 & 0 \\ & & & \dots & & \\ 0 & 0 & 0 & \dots & S_{q-1q-1} & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 \end{bmatrix}$$

such that

$$S\mathbf{d} = P^{-1}\mathbf{h} ,$$

or, equivalently,

$$S\mathbf{d} = \frac{1}{a\bar{\psi}} \bar{z}_{VN} ,$$

since, from Eq. (37),  $\mathbf{h} = \frac{1}{a\bar{\psi}} P\bar{z}_{VN}$ . The particular structure of  $S$  and  $\mathbf{d}$  turns out from Eq. (36b). Observe that  $S$  is non singular as it follows from the assumption that all perturbations of the state vector  $\mathbf{z}$  have an exponential time dependence.

The perturbation  $\bar{z}$  normalized with respect to the von Neumann state can be expressed by the  $q$ -component vector  $\mathbf{g}$  given by

$$(40) \quad \mathbf{g} = \frac{1}{\bar{\psi}} S^{-1}\bar{z} .$$

Note that the normalization (40) permits to avoid the dependence on  $\bar{\psi}$  in the linearized Euler equations (35). The value of  $\mathbf{g}$  at the von Neumann state is simply

$$(41) \quad \mathbf{g}_{VN} = a\mathbf{d} .$$

#### Linear stability equations in the steady reaction coordinate

The linearized Euler equations (35), with the reaction coordinate (38) and normalization (40), become

$$(42) \quad \frac{d\mathbf{g}}{ds} + [aF^*(\mathbf{z}^*; \mathcal{O}^l) + G^*(\mathbf{z}^*; \mathcal{O}^l)]\mathbf{g} + a\mathbf{y}^*(\mathbf{z}^*; \mathcal{O}^l) = \mathbf{0} ,$$

where the coefficient matrices depend now on the reaction coordinate  $s$ , and are given by

$$F^* = \frac{v_{B_1}^*}{r^*} S^{-1} (A^* - \mathcal{O}^l B^*)^{-1} B^* S$$

$$G^* = \frac{v_{B_1}^*}{r^*} S^{-1} (A^* - \mathcal{O}^l B^*)^{-1} \left[ \frac{r^*}{v_{B_1}} \mathbf{r}^T \frac{dz^*}{ds} (A_1 - \mathcal{O}^l B_1) - C_1 \right] S$$

$$\mathbf{y}^* = -S^{-1} (A^* - \mathcal{O}^l B^*)^{-1} B^* \frac{dz^*}{ds}.$$

### Initial conditions in the steady reaction coordinate

Referring the initial conditions (37) to the reaction coordinate (38) and normalization (40), one gets

$$(43) \quad \mathbf{g}(0) = a\mathbf{d},$$

since  $s = 0$  at the von Neumann state. Equations (43) are the initial conditions for Eqs. (42) in the reaction coordinate.

To conclude this section, let underline, once more, that the linear stability problem is formulated in the steady reaction coordinate  $s$  by means of the initial value problem (42)-(43), in terms of the complex disturbance  $\mathbf{g}$  and growth rate  $a$ .

## 5 - Determinacy of the stability problem

The initial-value problem (42)-(43) provides the  $s$ -evolution of the disturbances  $\mathbf{g}$  in the reaction zone, when the perturbation parameter  $a$  is assigned. Since  $a$  cannot be known *a priori*, this problem is, in general, not closed. Its determinacy is assured by an algebraic condition which constitutes the dispersion relation of the normal mode expansions (31).

As already mentioned at the beginning of section 4, such a constraint is derived assuming that the disturbances  $\mathbf{g}$  are not affected by subsequent rear perturbations, travelling towards the shock wave. This assumption is translated into a *radiation condition* through an acoustic analysis at the end of the reaction zone, as proposed by Lee & Stewart [6].

### 5.1 - Acoustics at the end of the reaction zone

The acoustic analysis is performed at the end of the reaction zone, where the gas flow is nearly in thermodynamical equilibrium conditions. Hence the reactive

Euler equations (23) are linearized using the approximation

$$(44) \quad \mathbf{z}(x, t) = \mathbf{z}_e^* + \mathbf{z}^{ac}(x, t),$$

where  $\mathbf{z}_e^*$  is the equilibrium steady solution to the Rankine-Hugoniot conditions (25) referred to the final state F, and  $\mathbf{z}^{ac}$  a small acoustic perturbation.

#### Acoustic equations

Insert expansion (44) in Eq. (23) and neglect the non linear terms with respect to  $\mathbf{z}^{ac}$ . The coefficient matrices  $B$ ,  $A$ ,  $\mathbf{c}$  can be then expanded in the form

$$(45) \quad \begin{aligned} B(\mathbf{z}) &= B_e^*(\mathbf{z}_e^*) + B_1(\mathbf{z}_e^*) \mathbf{z}^{ac} \mathbf{r}^T \\ A(\mathbf{z}) &= A_e^*(\mathbf{z}_e^*) + A_1(\mathbf{z}_e^*) \mathbf{z}^{ac} \mathbf{r}^T \\ \mathbf{c}(\mathbf{z}) &= \mathbf{c}_e^*(\mathbf{z}_e^*) + C_1(\mathbf{z}_e^*) \mathbf{z}^{ac}, \end{aligned}$$

where, as already mentioned,  $B_1$ ,  $A_1$ ,  $C_1$  are  $q$ -square matrices and  $\mathbf{r}^T = [1 \dots 1]$  is a  $q$ -row vector; moreover  $\mathbf{c}_e^*(\mathbf{z}_e^*) = 0$  since  $\mathbf{z}_e^*$  is the thermodynamical equilibrium steady solution. The reactive Euler equations (23) can be written as a set of partial linear differential equations with constant coefficients

$$(46) \quad \frac{\partial \mathbf{z}^{ac}}{\partial t} + E_e^* \frac{\partial \mathbf{z}^{ac}}{\partial x} + C_e^* \mathbf{z}^{ac} = 0,$$

where

$$(47) \quad E_e^* = (B_e^*)^{-1} A_e^*, \quad C_e^* = - (B_e^*)^{-1} C_1(\mathbf{z}_e^*).$$

The system (46), as shown in [9], results to be hyperbolic, thus it can be transformed into the canonical form, see the book [12], diagonalizing the matrix  $E_e^*$  through a similarity transformation  $R^{-1} E_e^* R$ , where  $R$  is the matrix whose columns are the eigenvectors of  $E_e^*$ . The resulting equations are

$$(48) \quad \frac{\partial \mathbf{v}^{ac}}{\partial t} + H_e^* \frac{\partial \mathbf{v}^{ac}}{\partial x} + J_e^* \mathbf{v}^{ac} = 0,$$

where

$$\mathbf{v}^{ac} = R^{-1} \mathbf{z}^{ac}, \quad H_e^* = R^{-1} E_e^* R, \quad J_e^* = R^{-1} C_e^* R.$$

Equations (48) are the acoustic equations of the model.

### Acoustic waves

Acoustic waves are achieved by means of a well known procedure, which is here applied. Normal mode solutions to (48) are searched in the form

$$(49) \quad \mathbf{v}^{ac}(x, t) = \mathbf{v}(k) \exp[ikx - \gamma(k)t],$$

where  $i = \sqrt{-1}$ ,  $\mathbf{v}(k)$  is a constant vector, the parameter  $k$  is assumed to be real and  $\gamma(k)$  has to be chosen in a fashion that (49) satisfies Eq. (48). Non trivial solutions of (48) correspond to the following condition of  $q$ -degree with respect to  $\gamma(k)$

$$(50) \quad \det(ikH_e^* - \gamma(k)I + J_e^*) = 0,$$

which constitutes the dispersion relation of the normal modes (49). The  $q$  roots of Eq. (50),  $\gamma_1(k), \dots, \gamma_q(k)$ , lead to the  $q$  elementary solutions to Eq. (48),  $\mathbf{v}_j^{ac}(x, t; k)$ , namely

$$(51) \quad \mathbf{v}_j^{ac}(x, t; k) = \mathbf{v}_j(k) \exp[ikx - \gamma_j(k)t], \quad j = 1, \dots, q.$$

Observe that each coefficient vector  $\mathbf{v}_j(k)$  is determined in a fashion that the vector function (51) satisfies Eq. (48).

A more convenient form of  $\mathbf{v}_j^{ac}$  is

$$(52) \quad \mathbf{v}_j^{ac}(x, t; k) = \mathbf{v}_j(k) \exp[i(kx - \text{Im } \gamma_j(k)t)] \exp(-\text{Re } \gamma_j(k)t), \quad j = 1, \dots, q,$$

which permits to identify the *wave number*  $k$ , *frequency*  $\text{Im } \gamma_j(k)$ , *phase*  $kx - \text{Im } \gamma_j(k)t$  and *phase velocity*  $[\text{Im } \gamma_j(k)]/k$ .

Thus, a formal solution to Eq. (48),  $\mathbf{v}^{ac}(x, t)$ , is obtained by Fourier superposition of the dispersive wave solutions

$$(53) \quad \mathbf{v}^{ac}(x, t; k) = \sum_{j=1}^q \mathbf{v}_j^{ac}(x, t; k), \quad k \in \mathbb{R}.$$

### Radiation condition

The afore-mentioned radiation condition means that no acoustic waves emanate from the rear boundary to interfere with the perturbed solution. In other words, the dispersive acoustic wave does not depend on the forward waves travelling towards the shock. Denote the forward phase velocity by  $[\text{Im } \gamma_1]/k$  and the corresponding wave by  $\mathbf{v}_1^{ac}$ ; the above requirement sets

$$(54) \quad \mathbf{v}_1^{ac}(x, t; k) = 0, \quad k \in \mathbb{R}.$$

The wave solution  $\mathbf{v}^{ac}(x, t; k)$ , given by expression (53) with condition (54), is then represented, at most, by  $q - 1$  linearly independent elementary solutions  $\mathbf{v}_2^{ac}(x, t; k), \dots, \mathbf{v}_q^{ac}(x, t; k)$ , defined by Eqs. (51). The same happens when one considers the Fourier superposition  $\mathbf{v}^{ac}(x, t)$ ; therefore, the set

$$\{\mathbf{v}^{ac}(x, t), \mathbf{v}_2^{ac}(x, t; k), \dots, \mathbf{v}_q^{ac}(x, t; k)\}$$

is linearly dependent. Accordingly the matrix, whose columns are the vectors of the above written set, is singular, namely

$$(55) \quad \det[\mathbf{v}^{ac}(x, t) \mathbf{v}_2^{ac}(x, t; k) \dots \mathbf{v}_q^{ac}(x, t; k)] = 0,$$

which constitutes an homogeneous algebraic constraint corresponding to the radiation condition.

### 5.2 - Dispersion relation for the stability equations

The above results, and in particular Eq. (55), will be now converted into the terminology of the stability problem. At this end, express the acoustic perturbation wave  $\mathbf{v}^{ac}(x, t)$  in terms of the growth rate  $a$  and disturbance  $\bar{\mathbf{z}}$ , through the equality

$$(56) \quad \mathbf{v}^{ac}(x, t) = \exp(at) \bar{\mathbf{z}}(x).$$

Moreover, express the acoustic wave number  $k$  in terms of  $a$ , identifying a normal mode, say  $\mathbf{v}_2^{ac}(x, t; k)$ , as

$$\mathbf{v}_2(k) \exp[ikx - \gamma_2(k) t] = \mathbf{v}_2(k) \exp(ikx) \exp(at).$$

It easily follows

$$(57) \quad a = -\gamma_2(k).$$

The algebraic constraint (55), with positions (56), (57) and normalization (40) of  $\bar{\mathbf{z}}$ , can be now converted into the stability nomenclature; the following manipulations on the columns of the matrix which figures in Eq. (55) will be performed:

- substitute the first column by  $\exp(at) \bar{\mathbf{z}}(x)$ ;
- replace the wave coordinate  $x$  by the steady reaction coordinate  $s$ , by means of (38);

- replace  $\bar{z}$  by the normalized disturbance  $\mathbf{g}$ , using Eq. (40), i.e.

$$\bar{z} = \bar{\psi} S \mathbf{g} ;$$

- express  $k$  as a function of  $a$  in all columns but the first one, by means of (57).

After that, condition (55) turns out to be equivalent to an algebraic equation which hereinafter will be indicated by

$$(58) \quad \mathcal{L}(a, \mathbf{g}) = 0 .$$

Observe that Eq. (58) holds at the equilibrium final state at the end of the reaction zone, where  $s = \lambda_e^*$ .

Equation (58) is the required dispersion relation associated to the normal mode expansions (31), needed to close the stability initial value problem (42)-(43).

## 6 - Conclusion

The linear stability problem of the steady detonation is stated in a closed form, in terms of the complex disturbance  $\mathbf{g}$  and growth rate  $a$ , by means of a set of ordinary differential equations with non constant coefficients

$$\frac{d\mathbf{g}}{ds} + aF^* \mathbf{g} + G^* \mathbf{g} + a\mathbf{y}^* = 0 , \quad s \in (0, \lambda_e^*) ,$$

with initial data assigned at the von Neumann state

$$\mathbf{g} = a\mathbf{d} , \quad \text{for } s = 0 ,$$

and dispersion relation

$$\mathcal{L}(a, \mathbf{g}) = 0 , \quad \text{for } s = \lambda_e^* .$$

Therefore, since  $\mathbf{g}$  and  $a$  are complex, the problem consists of  $2q$  differential equations subjected to  $2q$  shock conditions at  $s = 0$  plus two conditions at the equilibrium  $s = \lambda_e^*$ . Such last conditions must be regarded as the ones which allow to evaluate the complex number  $a$ .

The knowledge of  $a$  finally gives the responses of the steady detonation to the applied rear perturbations. In fact, the asymptotic behaviour of the perturbed detonation solution is determined by  $\text{Re } a$ , since the disturbances are given by  $\bar{\psi} \exp(at) S \mathbf{g}$ , as it immediately follows from Eqs. (31), (40).

The following criterion, based on the well known Lyapunov criterion, can so be enunciated.

*If the real part of  $a$  is negative, then the disturbances asymptotically decay in time and the steady solution is stable; otherwise the steady detonation solution is unstable.*

The linear stability problem, as above formulated, formally recovers the classical one treated in literature by Lee & Stewart [6]; the unknown vector  $\mathbf{g}$  here defines the disturbance of the microscopic state of the detonating gas.

In conclusion, the present paper should be regarded as a completion of the approach to steady detonation by means of discrete kinetic theory. It constitutes the analytical background for the numerical treatment of one-dimensional linear detonation stability, once the appropriate discrete model, describing the steady detonation wave structure, has been chosen. In other words, the detonation stability can actually be discussed in the framework of the extended kinetic theory, applying the general procedure here proposed, which constitutes the mathematical tool necessary to future applications. In fact, starting from the steady detonation solutions, numerically provided in papers [2] and [3], one can adapt, step by step, all the rather cumbersome items of sections 4 and 5 to a particular kinetic model. Thus, the stability behaviour of a detonating gas mixture with either bimolecular or autocatalytic reaction, needs to be studied, separately, in a forthcoming work.

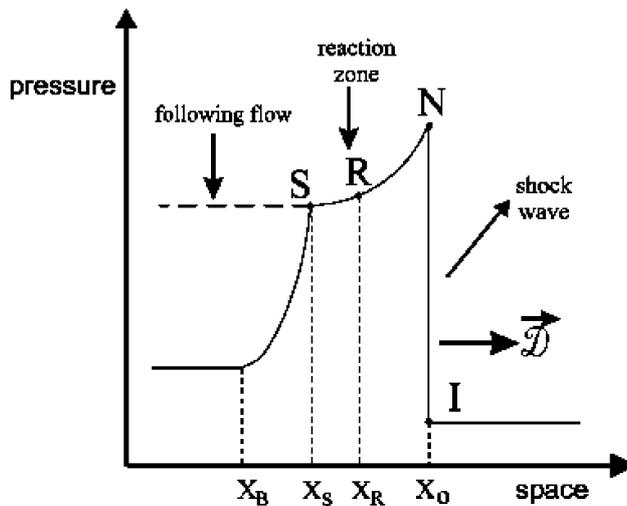


Figure 1 - ZND model-detonation with one reversible reaction.

### References

- [1] R. MONACO, M. PANDOLFI BIANCHI and A. J. SOARES, *Steady detonation waves in classical and discrete kinetic theory*, Comm. Appl. Nonlinear Anal. **3** (1996), 1-19.
- [2] M. PANDOLFI BIANCHI and A. J. SOARES, *A kinetic model for a reacting gas flow: steady detonation and speeds of sound*, Phys. Fluids **8** (1996), 3423-3432.
- [3] M. PANDOLFI BIANCHI and A. J. SOARES, *Solutions to steady detonation and linear stability in discrete kinetic theory*, in Rarefied Gas Dynamics, Eds. R. Brun, R. Campargue, R. Gatignol, J. C. Lengrand, Vol. **1**, 1999, 79-86.
- [4] W. FICKETT and W. C. DAVIS, *Detonation*, University of California, Berkeley 1979.
- [5] J. J. ERPENBECK, *Stability of steady-state equilibrium detonations*, Phys. Fluids **5** (1962), 604-614.
- [6] H. I. LEE and D. S. STEWART, *Calculation of linear detonation instability: one-dimensional instability of plane detonation*, J. Fluid Mech. **216** (1990), 103-132.
- [7] R. MONACO and L. PREZIOSI, *Fluid dynamical applications of the discrete Boltzmann equation*, World Scientific, Singapore 1991.
- [8] W. FICKETT, *Introduction to detonation theory*, University of California, Berkeley 1986.
- [9] M. PANDOLFI BIANCHI and A. J. SOARES, *Reactive Euler equations of discrete models with reversible reactions*, Contin. Mech. Thermodyn. **12** (2000), 53-67.
- [10] K. K. KUO, *Principles of combustion*, Wiley, New York 1986.
- [11] J. D. BUCKMASTER and J. NEVES, *One-dimensional detonation stability - the spectrum for infinite activation energy*, Phys. Fluids **31** (1988), 3571-3576.
- [12] S. GODOUNOV, *Équations de la Physique Mathématique*, Mir Publ., 1973.
- [13] G. B. WHITHAM, *Linear and nonlinear waves*, Wiley, New York 1974.

### Abstract

*Within discrete kinetic theory extended to chemically reacting gases, the linear stability problem is formulated for one-dimensional steady detonation waves with finite reaction zone. The stability equations are deduced in a general form with reference to a class of discrete kinetic models for several gases and one reversible chemical reaction. An acoustic analysis is performed at the thermodynamical equilibrium and a radiation condition is assumed in order to deduce the dispersion relation needed to make the stability equations solvable.*

\* \* \*