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Roe Linearization for the van der Waals Gas

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An extension of the Roe linearization method to nonideal gases is described and applied to the particular case of the van der Waals gas. A supplementary relation connecting the thermodynamic variables is introduced to decouple the evaluation of the intermediate velocity and total specific enthalpy from the determination of the intermediate density, needed in the Jacobian matrix of the linearization due to the general thermodynamic character of the gas. The density value is obtained by solving the supplementary equation, which involves the Roe average of velocity and enthalpy, and that in the case of the polytropic van der Waals gas is a third-order algebraic equation. Numerical results are shown including classical and nonclassical behaviour in one-dimensional shock tube problems.

Key Words: Roe linearization; dense gases; nonclassical waves; van der Waals gas.

CONTENTS

1. INTRODUCTION

The computation of compressible flows of a gas described by the van der Waals equation of state is a very active research area in the study of dense gas near the liquid–vapor saturation curve. In particular, the van der Waals gas is often taken as a simple model of BZT (Bethe, Zel'dovich, and Thompson) fluid to investigate negative shock waves and other phenomena

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related to negative nonlinearity. Some commercially available heat transfer fluids such as, for instance, FC-71 ($C_{18}F_{39}N$), FC-72 (C_6F_{14}), PP9 ($C_{11}F_{20}$), or PP11 ($C_{14}F_{24}$) are believed to possibly exhibit nonclassical waves near the liquid–vapor saturation curve. This anomalous behavior occurs when the *fundamental derivative of gas dynamics* introduced by Bethe [4]

$$\mathcal{G}(s, v) \stackrel{\text{def}}{=} -\frac{v}{2}\frac{\partial^2 P(s, v)}{\partial v^2} \bigg/ \frac{\partial P(s, v)}{\partial v}, \tag{1.1}$$

with $P, s,$ and v denoting pressure, entropy per unit mass and specific volume, respectively, becomes negative. Since $\partial P(s, v)/\partial v < 0$ for thermodynamic stability, the negative sign of $\mathcal{G}$ is associated with regions of the flow field in which the isentropes in the volume–pressure plane are not convex; therefore, the polytropic ideal gas approximation, which allows for convex isentropes only, is no longer acceptable. A flow field in which $\mathcal{G}(s, v)$ becomes negative results into a loss of the genuinely nonlinear character of acoustic waves and may lead to the formation of negative or mixed waves as described in the fundamental paper of Menikoff and Plohr [21]; a flow regime of this kind is said to be a *dense gas regime*.

Mixed and split waves may also be formed—irrespective of the sign of $\mathcal{G}$—when the fluid undergoes a phase change because of the kink of the isentropes at the phase transition boundary. However, the study of these two-phase phenomena falls outside the scope of the present work.

The existence of mixed waves in the dense gas regime does not allow a direct use of most of the standard numerical techniques for solving the compressible Euler equations, which were developed to deal with classical wave structures. Moreover, if an artificial viscosity method is employed, care must be taken in the selection of the proper trigger for the numerical dissipation operator; in fact, standard sensors based on the sign of pressure jumps may fail to detect a nonclassical isentropic compression and may consequently introduce a too-large numerical dissipation.

In the framework of numerical schemes for the Euler equations for dense gases, different approaches have been followed. Argrow [2] used a predictor–corrector scheme based on the Davis flux limited method [9] for the van der Waals gas, being mainly interested in the evaluation of more refined gas models. Rider and Bates [26] developed a Riemann solver with an explicit treatment of the nonconvexity of the isentropic curves. Müller and Voß [24] opened the way to the use the standard Godunov method by developing an exact Riemann solver which takes into account nonclassical gas behavior. In the present work, a new method is presented, which extends the upwind scheme proposed by Roe [27] for the ideal polytropic gas to dense gas models in general and to the polytropic van der Waals gas in particular.

It is well known that the linearization procedure of Roe's scheme is not uniquely determined when a real gas equation of state is taken into account. Most of the formulations of Roe's method developed to deal with a general equation of state [1, 7, 10, 12, 19, 33] may be described as linearizations in quasi-Jacobian form [23], where the thermodynamic pressure derivatives are considered as additional unknowns that provide sufficient degrees of freedom to make the solution of the linearization problem unique. The proposed method follows a different approach, in which a strictly Jacobian form is retained—thus ensuring the hyperbolic character of the linearized problem—while the density is raised to the role of the required additional unknown.

This paper is organized as follows. In Section 2, the ideal and van der Waals gas models are briefly recalled. In Section 3, the Euler equations for a general (possibly nonideal) gas are presented, and the influence of the fundamental derivative on the properties of characteristic fields is discussed. In Section 4, the standard Roe linearization for the ideal gas with constant specific heats (polytropic) is recalled, and extensions to other gas models are briefly described. In Section 5, the proposed linearization procedure is described discussing both its reduced form for a possibly nonpolytropic gas and its general form for nonideal gases. In Section 6, the linearization procedure is applied to the polytropic van der Waals gas, for which numerical results are given in Section 7. In the appendices, the details of the solution of the linearization problem according to the proposed formulation are given.

2. THE VAN DER WAALS MODEL OF DENSE GASES

In this section, the basic thermodynamic properties of the ideal gas and of the van der Waals gas are recalled. In particular, the expression of the fundamental derivative $\mathcal{G}$, whose negative sign is associated with anomalous behaviour, is given.

As is well known, for an *ideal gas* with only a chemical species, the *equation of state* (EOS) for the pressure P is

$$P(T, v) = \frac{RT}{v}, \tag{2.1}$$

where T is the temperature, v is the specific volume, and $R \overset{\text{def}}{=} \mathcal{R}/\mu_0$ is a gas-dependent constant, $\mathcal{R}$ is the universal gas constant, and μ_0 is the molecular weight.

To have a complete description of the thermodynamic properties of the gas, a second EOS for the internal energy $e = e(T, v)$ is needed. This equation has to be compatible with (2.1), since both equations are a consequence of a single fundamental relation $s = s(e, v)$, where s is the entropy per unit mass. The energy equation compatible with (2.1) is easily seen to be of the form

$$e(T, v) = f(T),$$

where $f(T)$ is an arbitrary function, which is related to the heat capacity at constant volume c_v by $c_v(T) \overset{\text{def}}{=} \partial e(T, v)/\partial T = f'(T)$; by thermodynamic stability, $f'(T) = c_v(T) > 0$.

From a physical viewpoint, the form of the function $f(T)$ comes from the statistical mechanics of the gas, including effects of its possible rotational and vibrational degrees of freedom (see Landau and Lifshitz [16]). In particular, if a classical (nonquantum) mechanical treatment is assumed, c_v is constant, as it is always the case for a monoatomic gas, and the gas is said to be *polytropic*. The resulting (complete) model of *polytropic ideal gas* reads

$$P(T, v) = \frac{RT}{v}, \qquad e(T, v) = c_v T + e_0, \tag{2.2}$$

where e_0 is the reference internal energy at zero temperature that will be neglected in the following, without loss of generality.

Let us now consider the fundamental derivative of gas dynamics $\mathcal{G}$ defined in (1.1). For a polytropic ideal gas, the isentropes in the v-P plane, $P/v^{\delta+1} = \text{constant}$, where

$\delta = R/c_v$, have always a positive curvature, so that $\mathcal{G} > 0$ and therefore no anomalous behavior can occur. The above can be proved by substituting the definition of the speed of sound, $c^2(s, v) = -v^2 \partial P(s, v)/\partial v$, into (1.1); namely,

$$\mathcal{G}(s, v) = \frac{v^3}{2c^2} \frac{\partial^2 P(s, v)}{\partial v^2}.$$

From the expression above and using $P(s, v) = \delta \exp[\delta(s - s_0)/R]/v^{\delta+1}$, the expression of the fundamental derivative for a polytropic ideal assumes the constant value

$$\mathcal{G}(s, v) = \frac{\delta}{2} + 1 > 0, \tag{2.3}$$

which is positive due to thermodynamic stability ($\delta = R/c_v > 0$).

The ideal model of dimensionless colliding atoms or molecules has been extended in 1873 by J. D. van der Waals [32] to take into account repulsive covolume effects and attractive intermolecular forces. The resulting model leads to a pressure EOS in the form

$$P(T, v) = \frac{RT}{v - b} - \frac{a}{v^2}, \tag{2.4}$$

where a and b are two (gas-dependent) constants, functions of the strength of intermolecular forces (only pair interactions of molecules are considered), and of the volume of the molecules, respectively. For $v \gg b$ and $P \gg a/v^2$, i.e., far from the saturation curve, the ideal gas model is recovered. The energy EOS compatible with (2.4) is found to be in the form [6]

$$e(T, v) = f(T) - \frac{a}{v},$$

where again $f(T)$ is an arbitrary function but for the thermodynamic stability condition $f'(T) \equiv c_v(T) > 0$. Here, we restrict our analysis to the polytropic van der Waals gas model, defined by setting $f(T) = c_v T$, with c_v a known constant, so that

$$e(T, v) = \frac{RT}{\delta} - \frac{a}{v}, \tag{2.5}$$

where again $\delta = R/c_v$. For completeness, we recall the expression of the fundamental relation for the polytropic van der Waals gas, namely,

$$s(e, v) = R \ln\left[(v - b)\left(e + \frac{a}{v}\right)^{\frac{1}{\delta}}\right] + s_0, \tag{2.6}$$

in which s_0 is a constant. From (2.4) and (2.6), we can write the EOS for the pressure as a function of the specific entropy and specific volume, namely,

$$P(s, v) = \delta \frac{\exp\left[\frac{\delta}{R}(s - s_0)\right]}{(v - b)^{\delta+1}} - \frac{a}{v^2}. \tag{2.7}$$

We notice in passing that the isentropes, which can be obtained from (2.7) by taking $s =$ constant, reduce to the ones obtained in the polytropic ideal case, i.e., $P/v^{\delta+1} =$ constant,

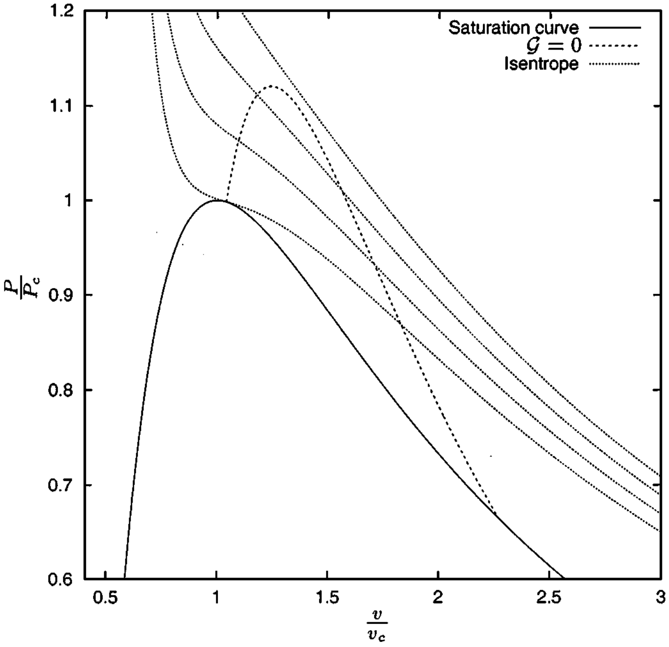

FIG. 1. Isentropes in the v-P plane for a van der Waals gas with $\delta = 0.0125$. The nonconvex region is located between the $\mathcal{G} = 0$ locus and the saturation curve. The critical point C has coordinates $v_c = 3b$, $P_c = a/27b^2$.

in the limit $v \to \infty$. Furthermore, in the limit $\delta \to 0$, the isentropes are coincident with the van der Waals isotherms.

From (2.4), the fundamental derivative of the van der Waals gas is easily obtained as

$$\mathcal{G}(P, v) \overset{\text{def}}{=} \mathcal{G}(s(P, v), v) = \frac{(\delta + 1)(\delta + 2)\frac{P + a/v^2}{(v-b)^2} - \frac{6a}{v^4}}{2(\delta + 1)\frac{P + a/v^2}{v(v-b)} - \frac{4a}{v^4}}, \tag{2.8}$$

which has been expressed[1] in terms of the pressure and specific volume for later convenience.

For the polytropic van der Waals gas a finite region of negative $\mathcal{G}$ may exist [29] in the vapor phase near the saturation curve (see Fig. 1). The locus $\mathcal{G} = 0$, the boundary between the classical and nonclassical regimes, can be found by setting the numerator of (2.8) to zero and solving for the pressure P to find

$$P_{\mathcal{G}=0}(v) = \frac{a}{v^2}\left[\frac{6}{(\delta + 1)(\delta + 2)}\left(1 - \frac{b}{v}\right)^2 - 1\right]. \tag{2.9}$$

In the limit $\delta \to 0$, i.e, $c_v \to \infty$, the locus $\mathcal{G} = 0$ is a line in the plane v-P starting from the critical point of coordinates ($v_c = 3b$, $P_c = a/27b^2$) and delimiting, together with the

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[1] Here and in the following, with a slight abuse of mathematical notation, we will denote different functions of a given physical quantity in terms of different variables by one and the same symbol, as it is a standard practice in thermodynamic formulae.

saturation curve, a finite region of negative $\mathcal{G}$ in the vapor phase. The extent of the nonclassical region diminishes as δ increases, and reduces to a single point on the saturation curve of coordinates $(1.4843v_c, 0.888P_c)$ for $\delta = \delta^* = 1/16.66 = 0.06$, as given by Thompson and Lambrakis [30]. Otherwise, if $\delta > \delta^*$, no anomalous behavior can be observed in the vapor phase. In Fig. 1, the nonclassical region is shown for $\delta = 0.0125$.

Thanks to this simple algebraic form, the polytropic van der Waals gas has been often used as a qualitative model to study the behavior of negative nonlinearities near the saturation curve [2, 3, 5, 8, 22, 24]. Nevertheless, more accurate models are available and are currently employed whenever a quantitative analysis is needed; see, for instance, the works of Reid, Prausnitz and Poling [25] and of Martin and Hou [20].

3. EULER EQUATIONS FOR NONIDEAL GASES

We now consider a system of conservation laws in one spatial dimension for the vector unknown $\boldsymbol{w}(x,t) \in \mathbb{R}^p$, $x \in \mathbb{R}$, $t > 0$, in the form

$$\frac{\partial \boldsymbol{w}}{\partial t} + \frac{\partial \boldsymbol{f}(\boldsymbol{w})}{\partial x} = 0, \tag{3.1}$$

where the flux $\boldsymbol{f}(\boldsymbol{w}) : \mathbb{R}^p \to \mathbb{R}^p$ is a given vector function. For the one-dimensional Euler equations of gasdynamics of interest here, we have

$$\boldsymbol{f}(\boldsymbol{w}) = \left(m,\ \frac{m^2}{\rho} + \Pi(\boldsymbol{w}),\ \frac{m}{\rho}(E^{\mathrm{t}} + \Pi(\boldsymbol{w}))\right)^{\mathrm{T}}, \tag{3.2}$$

where $\boldsymbol{w} = (\rho, m, E^{\mathrm{t}})^{\mathrm{T}} \in \Omega \subset [\mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}]$ is the vector of the conservative variables mass, momentum, and total (internal and kinetic) energy per unit volume. From the EOS $P = P(E, \rho)$, where E is the internal energy per unit volume, we have introduced the *pressure function* in terms of the conservative variables, namely,

$$\Pi(\boldsymbol{w}) \overset{\text{def}}{=} P\left(E^{\mathrm{t}} - \frac{m^2}{2\rho}, \rho\right). \tag{3.3}$$

For later convenience, we recall here the Jacobian matrix of the flux, $\boldsymbol{A}(w) = \partial \boldsymbol{f}(w)/\partial w$, namely,

$$\boldsymbol{A}(\boldsymbol{w}) = \begin{pmatrix} 0 & 1 & 0 \\ -\frac{m^2}{\rho^2} + \Pi_\rho(\boldsymbol{w}) & \frac{2m}{\rho} + \Pi_m(\boldsymbol{w}) & \Pi_{E^{\mathrm{t}}}(\boldsymbol{w}) \\ \frac{m}{\rho}\left(-\frac{E^{\mathrm{t}}+\Pi(\boldsymbol{w})}{\rho} + \Pi_\rho(\boldsymbol{w})\right) & \frac{E^{\mathrm{t}}+\Pi(w)}{\rho} + \frac{m}{\rho}\Pi_m(\boldsymbol{w}) & \frac{m}{\rho}(1 + \Pi_{E^{\mathrm{t}}}(\boldsymbol{w})) \end{pmatrix},$$

where we used the standard notation $\Pi_{w_k}(\boldsymbol{w}) \overset{\text{def}}{=} \partial \Pi(\boldsymbol{w})/\partial \boldsymbol{w}_k$, $k = 1, 2, 3$. The partial derivatives of $P(E, \rho)$ can be easily obtained from those of $\Pi(\boldsymbol{w})$ by means of the chain rule as

$$\frac{\partial P(E,\rho)}{\partial E} = \Pi_{E^{\mathrm{t}}}(\boldsymbol{w}), \quad \frac{\partial P(E,\rho)}{\partial \rho} = \Pi_\rho(\boldsymbol{w}) - \frac{1}{2}\frac{m^2}{\rho^2}\Pi_{E^{\mathrm{t}}}(\boldsymbol{w}), \tag{3.4}$$

where the variable E on the left-hand sides is to be expressed in terms of the conservative variables $\boldsymbol{w}$ through the relation $E = E(\boldsymbol{w}) = E^{\mathrm{t}} - m^2/(2\rho)$. Moreover, $P(E, \rho)$ being a function of only two variables, the following relation holds:

$$\Pi_m(\boldsymbol{w}) = -\frac{m}{\rho}\Pi_{E^{\mathrm{t}}}(\boldsymbol{w}). \tag{3.5}$$

Let us briefly recall some properties of the characteristic fields of the Euler equations in one dimension which are peculiar to the dense gas regime. For a complete description, we refer to the review of Menikoff and Plohr [21] and to the recent work of Müller and Voß [24]. For the kth characteristic fields, we introduce the *nonlinearity factor*

$$\alpha_k(\boldsymbol{w}) \overset{\text{def}}{=} \boldsymbol{\nabla}_{w}\lambda_k(\boldsymbol{w}) \cdot \boldsymbol{r}_k(\boldsymbol{w}), \tag{3.6}$$

where $\lambda_k(\boldsymbol{w}) = m/\rho + \varepsilon_k c(\boldsymbol{w})$, $\varepsilon_k = k - 2$, $k = 1, 2, 3$, and $\boldsymbol{r}_k(\boldsymbol{w})$ are the eigenvalues and the eigenvectors of the Jacobian matrix $\boldsymbol{A}(\boldsymbol{w})$, respectively, $c(\boldsymbol{w})$ is the speed of sound and $\boldsymbol{\nabla}_w \overset{\text{def}}{=} \partial/\partial\boldsymbol{w}$.

As is well known, the value of the nonlinearity parameter is of the utmost importance in classifying characteristic fields. The kth characteristic field is said to be *linearly degenerate* if $\alpha_k(\boldsymbol{w}) = 0\,\forall\boldsymbol{w} \in \Omega$, while if $\alpha_k(\boldsymbol{w}) \neq 0\ \forall\boldsymbol{w} \in \Omega$, the characteristic field is said to be *genuinely nonlinear* (see, for instance, Godlewski and Raviart [11]). Let us now clarify the consequences of the sign of the fundamental derivative in the definition of the characteristic fields, by writing the nonlinearity factor in the equivalent form [21]

$$\alpha_k(\boldsymbol{w}) = \varepsilon_k \mathcal{G}(\boldsymbol{w}) c(\boldsymbol{w}) \rho, \tag{3.7}$$

where again the notation $\mathcal{G}(\boldsymbol{w})$ implies the change of variables $(s, v) \to \boldsymbol{w}$. In the theory of ideal polytropic gases, $\mathcal{G} = \text{const} > 0$, so that both the first and the third fields ($\varepsilon_1 = -1$, $\varepsilon_3 = 1$) are genuinely nonlinear and classical compressive shocks and rarefaction fans are observed. The second characteristic field ($\varepsilon_2 = 0$) is instead linearly degenerate, and it is associated with contact discontinuities. Such a hyperbolic system, for which characteristic fields are either genuinely nonlinear or linearly degenerate, is called a *convex* hyperbolic system.

On the contrary, in the dense gas regime in the locus $\mathcal{G} = 0$ (Fig. 1), we have $\alpha_k(\boldsymbol{w}) = 0$, $k = 1, 2, 3$, and the genuine nonlinearity is lost. Consequently, the hyperbolic system is *nonconvex* and nonclassical negative or mixed waves can possibly occur. An example is given in Fig. 2, where the density distribution resulting from a shock tube problem is shown together with the locus of the gas states in the v-P plane. Both left and right initial states lie in the positive $\mathcal{G}$ region, but during the time evolution the gas states cross the $\mathcal{G} = 0$ boundary. Together with a classical compressive shock and a contact discontinuity propagating toward the low pressure side, the flow is characterized by a mixed rarefaction wave where the rarefaction fan moving toward the pressure side is connected with a rarefaction shock. For the description of the mathematical difficulties arising from considering this kind of nonclassical Riemann problems and for their solution, we refer again to [21] and [24].

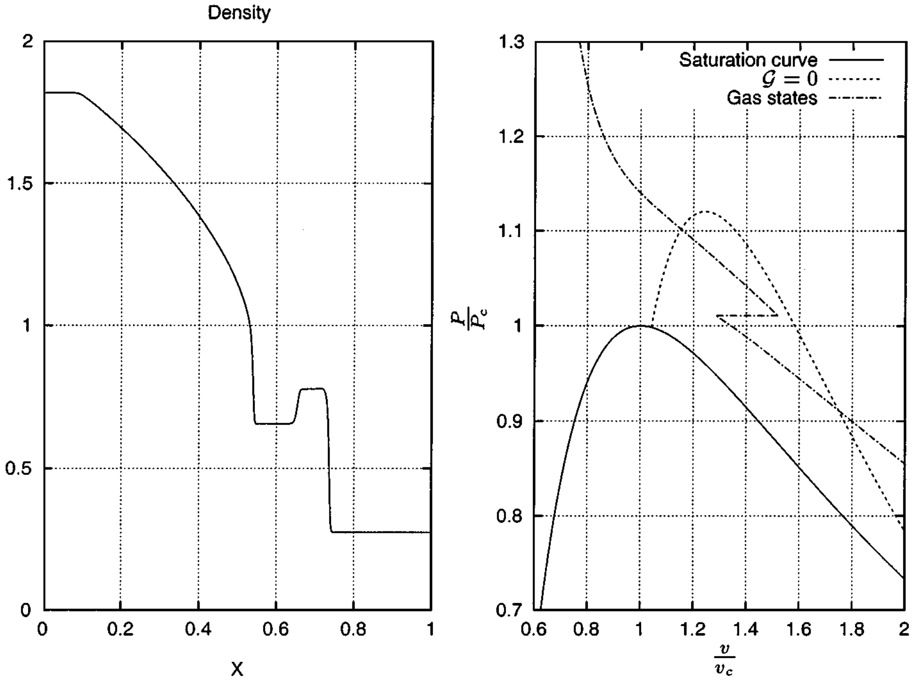

FIG. 2. Example of a mixed rarefaction wave. Density distribution (left) and gas states in the v-P plane (right). The dotted line is the boundary of the nonclassical region.

4. ROE LINEARIZATION

As is well known, Roe's Approximate Riemann Solver (ARS) is a Godunov-type scheme based on a local linearization of the considered hyperbolic system of conservation laws, devised in order to avoid the exact solution of Riemann problems [27]. For a detailed description of the method (and of its higher order implementation), we refer to LeVeque's [18] and Godlewski and Raviart's [11] monographs.

Let us consider the solution of the Riemann problem associated with the left and right states w_ℓ and w_r, namely,

$$\begin{cases} \dfrac{\partial \boldsymbol{w}}{\partial t} + \dfrac{\partial \boldsymbol{f}(\boldsymbol{w})}{\partial x} = 0, \\ \boldsymbol{w}(x,0) = \begin{cases} \boldsymbol{w}_\ell & x < 0 \\ \boldsymbol{w}_r & x > 0 \end{cases} \end{cases}$$

by means of the Roe linearization technique. The conservation law is approximated by a linearized equivalent substitute as

$$\frac{\partial \boldsymbol{w}}{\partial t} + \boldsymbol{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r)\frac{\partial \boldsymbol{w}}{\partial x} = 0, \tag{4.1}$$

where a suitable matrix $\boldsymbol{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r)$ of dimension $p \times p$ (function of the left and right state $\boldsymbol{w}_\ell$ and $\boldsymbol{w}_r$) has been introduced, according to the following prescriptions:

DEFINITION 4.1. Matrix $\boldsymbol{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r)$ is called a Roe linearization of the hyperbolic system with flux $\boldsymbol{f}(\boldsymbol{w})$ and Jacobian matrix $\boldsymbol{A}(\boldsymbol{w}) = \partial \boldsymbol{f}(\boldsymbol{w})/\partial \boldsymbol{w}$ if $(\boldsymbol{w}_\ell, \boldsymbol{w}_r) \to \boldsymbol{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r)$ is a mapping from $\mathbb{R}^p \times \mathbb{R}^p$ into the set of $p \times p$ matrices with the following properties:

(i) Conservation: $\boldsymbol{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r)(\boldsymbol{w}_r - \boldsymbol{w}_\ell) = \boldsymbol{f}(\boldsymbol{w}_r) - \boldsymbol{f}(\boldsymbol{w}_\ell)$,

(ii) Hyperbolicity: $\boldsymbol{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r)$ has real eigenvalues and a corresponding set of eigenvectors that form a basis of $\mathbb{R}^p$,

(iii) Consistency: $\boldsymbol{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r) \to \boldsymbol{A}(\boldsymbol{w})$ as $\boldsymbol{w}_\ell$ and $\boldsymbol{w}_r \to w$.

In principle, the determination of the *Roe matrix* $\mathbf{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r)$ satisfying the conditions above requires the definition of all its $p \times p$ elements $a^*_{i,j}(\boldsymbol{w}_\ell, \boldsymbol{w}_r)$, which are related by the p quantitative conditions stated in (i), assuming that conditions (ii) and (iii) are satisfied. If the p conditions are all nontrivial, the general solution for the linearization matrix will be a $(p^2 - p)$-parameter family of solutions. In particular, for the Euler equations in one spatial dimension, $p = 3$, and we have a six-parameter family of solutions. In practice, to fulfill conditions (ii) and (iii), it is convenient to properly select the form of matrix $\boldsymbol{A}^*$. In the following sections, standard Roe matrices for the Euler equations are recalled for different gas models.

4.1. Roe Linearization for the Ideal Polytropic Gas

Originally, Roe ARS was formulated considering the Euler equations for a polytropic ideal gas through a suitable change of variables, i.e., the so-called parameter vector transformation [27]. In this case, the linearizing matrix is found to be equivalent to the Jacobian matrix of the flux function evaluated at an intermediate state $\tilde{w}(w_\ell, w_r)$, defined by Roe averaged values of velocity $\tilde{u}$ and total specific enthalpy $\widetilde{h^{\rm t}}$, while no intermediate density is needed in the evaluation of the Jacobian matrix due to the particular form of the equations of state of the gas.

Denoting with $\boldsymbol{A}(\boldsymbol{w})$ the Jacobian matrix of the nonlinear hyperbolic system, a linearizing matrix of the form

$$\boldsymbol{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r) = \boldsymbol{A}(\tilde{\boldsymbol{w}}(\boldsymbol{w}_\ell, \boldsymbol{w}_r)) \tag{4.2}$$

will be called hereinafter a linearization in *Jacobian form*. For an ideal polytropic gas, this matrix can be defined in terms of only two variables, thanks to the first-order homogeneity of the flux function $\boldsymbol{f}(\boldsymbol{w})$. These two variables are typically chosen as the velocity and total specific enthalpy, so that

$$\boldsymbol{A}^*(\boldsymbol{w}_r, \boldsymbol{w}_\ell) = \boldsymbol{A}^{\rm PI}(\tilde{u}, \widetilde{h^{\rm t}}) = \begin{pmatrix} 0 & 1 & 0 \\ (\delta - 2)\tilde{u}^2 & \delta\tilde{u} & \delta \\ \tilde{u}\left(\frac{1}{2}\delta\tilde{u}^2 - \widetilde{h^{\rm t}}\right) & \widetilde{h^{\rm t}} - \delta\tilde{u}^2 & (\delta + 1)\tilde{u} \end{pmatrix}. \tag{4.3}$$

Solving now the linearization problem implied by condition (i), which now reads

$$\boldsymbol{A}^{\rm PI}(\tilde{u}, \widetilde{h^{\rm t}})(\boldsymbol{w}_r - \boldsymbol{w}_\ell) = \boldsymbol{f}(\boldsymbol{w}_r) - \boldsymbol{f}(\boldsymbol{w}_\ell),$$

we obtain the intermediate values of the velocity and total specific enthalpy, which are given by the celebrated expressions [27]:

$$\tilde{u} = \frac{\sqrt{\rho_\ell}u_\ell + \sqrt{\rho_r}u_r}{\sqrt{\rho_\ell} + \sqrt{\rho_r}}, \qquad \widetilde{h^{\rm t}} = \frac{\sqrt{\rho_\ell}h^{\rm t}_\ell + \sqrt{\rho_r}h^{\rm t}_r}{\sqrt{\rho_\ell} + \sqrt{\rho_r}}. \tag{4.4}$$

For the solution of the linearization problem using the direct substitution procedure outlined above, we refer, for example, to Mottura *et al.* [23] or to Guardone *et al.* [14].

4.2. Standard Extensions to Different Gas Models

To extend Roe solver to gas models different from the ideal polytropic one, several approaches have been followed [1, 7, 10, 12, 19, 33]. It has been noticed [23] that all these methods can be written so as to obtain a *quasi-Jacobian form* for the Roe matrix, in which the original intermediate state $(\tilde{u}, \widetilde{h^{\mathrm{t}}})$ of Roe is augmented by additional unknowns, namely, the pressure derivatives (either with respect to the conservative variables or with respect to two independent thermodynamic variables). The standard average for the velocity and total specific enthalpy can be recovered if the additional variables satisfy a linear relationship that will be given later on. The resulting *extended* intermediate state is not uniquely determined by applying the original parameter vector transformation and therefore, in most of these extensions, a defined intermediate state is singled out by directly imposing an additional constraint on the average pressure derivatives.

Let us consider the following quasi-Jacobian form of the Roe matrix, namely,

$$\begin{aligned}\boldsymbol{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r) &= \boldsymbol{A}^{\mathrm{qJ}}(\tilde{u}, \widetilde{h^{\mathrm{t}}}, \tilde{\Pi}_\rho, \tilde{\Pi}_m, \tilde{\Pi}_{E^{\mathrm{t}}}) \\ &= \begin{pmatrix} 0 & 1 & 0 \\ -\tilde{u}^2 + \tilde{\Pi}_\rho & 2\tilde{u} + \tilde{\Pi}_m & \tilde{\Pi}_{E^{\mathrm{t}}} \\ \tilde{u}(\tilde{\Pi}_\rho - \widetilde{h^{\mathrm{t}}}) & \widetilde{h^{\mathrm{t}}} + \tilde{u}\tilde{\Pi}_m & \tilde{u}(1 + \tilde{\Pi}_{E^{\mathrm{t}}}) \end{pmatrix}.\end{aligned} \tag{4.5}$$

This matrix is said to be in a quasi-Jacobian form since it is obtained from matrix $\boldsymbol{A}(\boldsymbol{w})$ in which the averaged quantities $\tilde{\Pi}_\rho$, $\tilde{\Pi}_m$, and $\tilde{\Pi}_{E^{\mathrm{t}}}$ are no longer the partial derivatives of $\Pi(\boldsymbol{w})$ evaluated in some intermediate state, but only additional parameters of the linearization procedure. In other words, matrix $\boldsymbol{A}^{\mathrm{qJ}}$ is uniquely determined by specifying an *extended* intermediate state $(\tilde{u}, \widetilde{h^{\mathrm{t}}}, \tilde{\Pi}_\rho, \tilde{\Pi}_m, \tilde{\Pi}_{E^{\mathrm{t}}})$. Assuming now the standard average (4.4) for the velocity and total specific enthalpy, it can be shown [23] that the two nontrivial equations stemming from the imposition of condition (i) are linearly dependent and reduce to the following single linear equation for the parameters $\tilde{\Pi}_\rho$, $\tilde{\Pi}_m$ and $\tilde{\Pi}_{E^{\mathrm{t}}}$

$$\tilde{\Pi}_\rho \Delta\rho + \tilde{\Pi}_m \Delta m + \tilde{\Pi}_{E^{\mathrm{t}}} \Delta E^{\mathrm{t}} = \Delta P, \tag{4.6}$$

where $\Delta(\cdot) = (\cdot)_r - (\cdot)_\ell$. Therefore, the solution of the linearization problem in a quasi-Jacobian form is a two-parameter family of solutions. In practice, to enforce consistency, relation (3.5) is imposed between $\tilde{u}$, $\tilde{\Pi}_m$, and $\tilde{\Pi}_{E^{\mathrm{t}}}$, to give the additional equation

$$\tilde{\Pi}_m = -\tilde{u}\tilde{\Pi}_{E^{\mathrm{t}}}, \tag{4.7}$$

thus reducing the number of degrees of freedom to one. Different methods are obtained according to different choices of the remaining parameter, as reviewed in [23].

The schemes based on the quasi-Jacobian form have proved successful in the computation of chemically reacting hypersonic flows and in different real gas applications. On the other hand, in our opinion, a drawback of these schemes lies in that the intermediate quantities $\tilde{\Pi}_\rho$, $\tilde{\Pi}_m$, and $\tilde{\Pi}_{E^{\mathrm{t}}}$ are artificial unknowns not retaining their exact thermodynamic significance: as pointed out by Toumi [31], this may lead to inconsistencies whenever these quantities are employed to derive other thermodynamic quantities such as, for example, the speed of sound, which is needed to evaluate the eigenstructure of the linear system. Moreover, in this approach conditions (ii) and (iii) still remain to be verified and in general their fulfillment will lead to additional constraints.

A noticeable exception is the work of Toumi [31], who, through a weak formulation of the linearization problem and by using a parameter vector approach, was able to obtain a simpler quasi-Jacobian form. In this approach the pressure derivatives are given in terms of an average Grüneisen coefficient, which is the only additional parameter with respect to the Jacobian approach. The latter quantity, approximated by numerical quadrature in state space, uniquely defines the Roe matrix, together with $\tilde{u}$ and $\widetilde{h^{\mathrm{t}}}$.

5. THE PROPOSED LINEARIZATION FOR NONIDEAL GASES

To overcome the difficulties highlighted in the previous section, we propose an extension of Roe ARS based on a strictly *Jacobian form*, by choosing $\boldsymbol{A}^*$ as the Jacobian matrix $\boldsymbol{A}(\boldsymbol{w}) = \partial \boldsymbol{f}(\boldsymbol{w})/\partial \boldsymbol{w}$ to be evaluated in an *intermediate state* $\tilde{\boldsymbol{w}} = \tilde{\boldsymbol{w}}(\boldsymbol{w}_\ell, \boldsymbol{w}_r)$ obtained from condition (i), which therefore becomes

$$\boldsymbol{A}(\tilde{\boldsymbol{w}}(\boldsymbol{w}_\ell, \boldsymbol{w}_r))(\boldsymbol{w}_r - \boldsymbol{w}_\ell) = \boldsymbol{f}(\boldsymbol{w}_r) - \boldsymbol{f}(\boldsymbol{w}_\ell), \tag{5.1}$$

and represents a system of p equations in the p unknowns $\tilde{w}_k$, $1 \le k \le p$. Such a Jacobian form ensures that the qualitative condition (ii) is automatically fulfilled and implies that condition (iii) now reads more simply: $\tilde{\boldsymbol{w}}(\boldsymbol{w}_\ell, \boldsymbol{w}_r) \to \boldsymbol{w}$ as $\boldsymbol{w}_\ell$ and $\boldsymbol{w}_r \to \boldsymbol{w}$.

Let us now particularize system (5.1) to the Euler equations. In this case, the Roe matrix $\boldsymbol{A}^*(\boldsymbol{w}_\ell, \boldsymbol{w}_r) = \boldsymbol{A}(\tilde{\boldsymbol{w}}(\boldsymbol{w}_\ell, \boldsymbol{w}_r))$ reads

$$\boldsymbol{A}(\tilde{\boldsymbol{w}}) = \begin{pmatrix} 0 & 1 & 0 \\ -\frac{\tilde{m}^2}{\tilde{\rho}^2} + \Pi_\rho(\tilde{\boldsymbol{w}}) & \frac{2\tilde{m}}{\tilde{\rho}} + \Pi_m(\tilde{\boldsymbol{w}}) & \Pi_{E^{\mathrm{t}}}(\tilde{\boldsymbol{w}}) \\ \frac{\tilde{m}}{\tilde{\rho}}\left(-\frac{\widetilde{E^{\mathrm{t}}} + \Pi(\tilde{\boldsymbol{w}})}{\tilde{\rho}} + \Pi_\rho(\tilde{\boldsymbol{w}})\right) & \frac{\widetilde{E^{\mathrm{t}}} + \Pi(\tilde{\boldsymbol{w}})}{\tilde{\rho}} + \frac{\tilde{m}}{\tilde{\rho}}\Pi_m(\tilde{\boldsymbol{w}}) & \frac{\tilde{m}}{\tilde{\rho}}(1 + \Pi_{E^{\mathrm{t}}}(\tilde{\boldsymbol{w}})) \end{pmatrix},$$

and the system (5.1) has three equations in the three unknowns $\tilde{\rho}$, $\tilde{m}$, $\widetilde{E^{\mathrm{t}}}$. The first equation of this system is identically satisfied ($\Delta m = \Delta m$) so that there are only two nontrivial equations and consequently the intermediate state is actually a one-parameter family of solutions. The two nontrivial equations stemming from the system can be rearranged so as to put in evidence the pressure jump and the partial derivatives of the function $\Pi(\boldsymbol{w})$ as

$$\begin{cases} (\Delta\rho)\left(\dfrac{\tilde{m}}{\tilde{\rho}}\right)^2 - 2(\Delta m)\dfrac{\tilde{m}}{\tilde{\rho}} + \Delta\dfrac{m^2}{\rho} + [\Delta P - \boldsymbol{\nabla}_w \Pi(\tilde{\boldsymbol{w}}) \cdot \Delta\boldsymbol{w}] = 0, \\ -(\Delta\rho)\dfrac{\tilde{m}}{\tilde{\rho}}\dfrac{\widetilde{E^{\mathrm{t}}} + \Pi(\tilde{w})}{\tilde{\rho}} + (\Delta m)\dfrac{\widetilde{E^{\mathrm{t}}} + \Pi(\tilde{\boldsymbol{w}})}{\tilde{\rho}} + (\Delta E^{\mathrm{t}})\dfrac{\tilde{m}}{\tilde{\rho}} + \dfrac{\tilde{m}}{\tilde{\rho}}\nabla_w \Pi(\tilde{\boldsymbol{w}}) \cdot \Delta\boldsymbol{w} \\ \qquad = \Delta\left(\dfrac{m}{\rho}(E^{\mathrm{t}} + \Pi)\right), \end{cases} \tag{5.2}$$

where $\Delta P = \Pi(\boldsymbol{w}_r) - \Pi(\boldsymbol{w}_\ell)$. This is a system of two coupled equations in the three unknowns $\tilde{\rho}$, $\tilde{m}$, $\widetilde{E^{\mathrm{t}}}$.

In the following sections, the solution of the linearization problem in Jacobian form will be analyzed; a distinction will be made between flux functions homogeneous of degree one, namely, under the hypothesis of gas ideality (Section 5.1), and flux functions stemming from a general nonideal gas (Section 5.2).

5.1. Ideal Gases and Homogeneity

Let us consider the case of a flux $\boldsymbol{f}(\boldsymbol{w})$ homogeneous of degree one with respect to $\boldsymbol{w}$. In this case, the equation system (5.1), which involves the evaluation of partial derivatives of $\boldsymbol{f}(\boldsymbol{w})$ only, can be written as a system in only $p-1$ unknowns, the usual choice for the Euler equations ($p=3$) being the velocity and total enthalpy per unit mass (u, h^{t}). As is well known [28], the above property of $\boldsymbol{f}(\boldsymbol{w})$ depends only on the thermodynamic model employed: in particular, $\boldsymbol{f}(\boldsymbol{w})$ is homogeneous of degree one if and only if the gas is ideal, irrespective of its polytropic or nonpolytropic character. In this case, for any equation of state $P(E,\rho)$, compatible with the assumption of gas ideality, the intermediate state $(\tilde{u}, \widetilde{h^{\mathrm{t}}})$ turns out to be uniquely determined as solution of the system of two equations (5.2). Under the further assumption of a *polytropic* gas, $P(E,\rho)=\delta E$ and the unique solution is provided by the so-called Roe average (4.4), which uniquely defines $\boldsymbol{A}^{\star}$ as in (4.3), while the intermediate state $\tilde{\boldsymbol{w}}$ of the conservative variables is defined up to an arbitrary density, for example.

On the contrary, for a *nonpolytropic* ideal gas, i.e., an ideal gas with a *nonlinear* function $e=f(T)$, the intermediate state is still defined uniquely as the solution of system (5.1), but in a way that in principle cannot be reduced to the Roe average (4.4) and that depends on the form of the function $f(T)$.

To conclude, we notice that the above holds also for gas models which differ from the ideal one by the occurrence of only an additive linear function of ρ in the EOS $P=P(E,\rho)$, since this dependency on ρ is eliminated by taking the derivative. This occurs for example for the stiffened Grüneisen equation of state [21], namely,

$$P(E,\rho)=\delta E+c_{\mathrm{ref}}^{2}(\rho-\rho_{\mathrm{ref}}),$$

where c_{ref} and ρ_{ref} are constant reference values, and an EOS which is obtained by linearizing a Grüneisen equation for a metal.

5.2. Nonideal Gases: An Equation for the Intermediate Density

Coming now to the nonideal gases of interest here, we propose to exploit the available degree of freedom of the one-parameter family of solutions of the linearization problem by fixing the intermediate state to reduce the complexity of system (5.2). This can be achieved by augmenting system (5.2) with the introduction of the *supplementary equation* [14]

$$\boxed{\boldsymbol{\nabla}_{w}\Pi(\tilde{\boldsymbol{w}})\cdot\Delta\boldsymbol{w}=\Delta P,} \tag{5.3}$$

so that we obtain the system

$$\begin{cases} \nabla_{w}\Pi(\tilde{w})\cdot\Delta w = \Delta P, \\ \dfrac{\tilde{m}}{\tilde{\rho}} = \dfrac{\frac{m_\ell}{\sqrt{\rho_\ell}} + \frac{m_r}{\sqrt{\rho_r}}}{\sqrt{\rho_\ell}+\sqrt{\rho_r}}, \\ \dfrac{\tilde{E}^{\mathrm{t}} + \Pi(\tilde{w})}{\tilde{\rho}} = \dfrac{\frac{E^{\mathrm{t}}_\ell + \Pi(w_\ell)}{\sqrt{\rho_\ell}} + \frac{E^{\mathrm{t}}_r + \Pi(w_r)}{\sqrt{\rho_r}}}{\sqrt{\rho_\ell}+\sqrt{\rho_r}}, \end{cases} \tag{5.4}$$

of three equations in the three unknowns $(\tilde{\rho}\tilde{m}, \widetilde{E^{\mathrm{t}}}) = \tilde{w}$. The augmented system (5.4) has been presented in [14] and its derivation is detailed in Appendix A. By introducing the variables velocity $u = m/\rho$ and total enthalpy per unit mass $h^{\mathrm{t}} = (E^{\mathrm{t}} + \Pi(w))/\rho$, that is, through the change of variable $w = (\rho, m, E^{\mathrm{t}}) \to v = (\rho, u, h^{\mathrm{t}})$, the second and third equations in (5.4) are solved to give explicit expressions for the intermediate velocity and total enthalpy in the form

$$\tilde{u} = \frac{\sqrt{\rho_\ell}u_\ell + \sqrt{\rho_r}u_r}{\sqrt{\rho_\ell}+\sqrt{\rho_r}} \quad \text{and} \quad \widetilde{h^{\mathrm{t}}} = \frac{\sqrt{\rho_\ell}h^{\mathrm{t}}_\ell + \sqrt{\rho_r}h^{\mathrm{t}}_r}{\sqrt{\rho_\ell}+\sqrt{\rho_r}}, \tag{5.5}$$

exactly as in the case of the polytropic ideal gas, while the introduced supplementary equation, written in terms of the new vector unknown $v = (\rho, u, h^{\mathrm{t}})$, is found to be an equation for the single unknown intermediate density $\tilde{\rho}$.

Summarizing, for any gas different from the ideal gas, the solution of the augmented linearization problem is obtained from the Roe-averaged quantities in (5.5) and from the subsequent solution of the single equation

$$\boxed{\nabla_{w}\Pi(w(\tilde{\rho}, \tilde{u}, \widetilde{h^{\mathrm{t}}}))\cdot\Delta w = \Delta P} \tag{5.6}$$

for the unknown $\tilde{\rho}$.

Let us now rewrite the supplementary equation (5.6) in a more convenient form. By using $\Delta E^{\mathrm{t}} - \Delta E = -\frac{1}{2}\Delta(m^2/\rho)$ and the fact that the intermediate velocity $\tilde{u}$ satisfies the following relation (from the momentum equation of the linearization problem, see Appendix A):

$$\Delta\left(\frac{m^2}{\rho}\right) = -\tilde{u}^2\Delta\rho + 2\tilde{u}\Delta m,$$

and by substituting relations (3.4) and (3.5) into Eq. (5.6), the supplementary equation assumes the form

$$\boxed{\frac{\partial P(\tilde{E}, \tilde{\rho})}{\partial E}\Delta E + \frac{\partial P(\tilde{E}, \tilde{\rho})}{\partial \rho}\Delta\rho = \Delta P} \tag{5.7}$$

having introduced the shorthand $\tilde{E} = E(\tilde{h}, \tilde{\rho}) = \tilde{\rho}\tilde{h} - P(\tilde{h}, \tilde{\rho})$ and $\tilde{h} = \widetilde{h^{\mathrm{t}}} - \tilde{u}^2/2$. Equation (5.7) makes explicit that the supplementary equation has a mere thermodynamic content. The complete system for the intermediate state $(\tilde{\rho}, \tilde{u}, \widetilde{h^{\mathrm{t}}})$ now reads,

$$\begin{cases} \tilde{u} = \dfrac{\sqrt{\rho_\ell}u_\ell + \sqrt{\rho_r}u_r}{\sqrt{\rho_\ell}+\sqrt{\rho_r}}, \qquad \widetilde{h^{\mathrm{t}}} = \dfrac{\sqrt{\rho_\ell}h^{\mathrm{t}}_\ell + \sqrt{\rho_r}h^{\mathrm{t}}_r}{\sqrt{\rho_\ell}+\sqrt{\rho_r}}, \\ \begin{cases} \frac{\partial P(\tilde{E},\tilde{\rho})}{\partial E}\Delta E + \frac{\partial P(\tilde{E},\tilde{\rho})}{\partial \rho}\Delta\rho = \Delta P, \\ \frac{\tilde{E}+P(\tilde{E},\tilde{\rho})}{\tilde{\rho}} = \widetilde{h^{\mathrm{t}}} - \frac{\tilde{u}^2}{2}, \end{cases} \end{cases} \tag{5.8}$$

where the definition of the internal energy $\tilde{E}$ has been written explicitly to have a closed system.

We want to stress again the fact that in the present method no averaging of the pressure derivatives is introduced, since their *analytical expressions* are evaluated exactly at the intermediate state, which is completely determined. Although the supplementary equation (5.3) takes a form similar to condition (4.6) needed in the quasi-Jacobian linearization, the two procedures are basically different. In fact, in a Roe linearization in quasi-Jacobian form, the extended intermediate state is found by imposing a a constraint on the *unknown* average derivatives of the pressure and the resulting linearization depends on the (arbitrary) average chosen for the pressure derivatives themselves. On the contrary, the supplementary equation introduced in the present approach selects a unique $\tilde{\boldsymbol{w}}$ within the one-parameter family of intermediate states and, at the same time, uncouples the determination of the unknowns intermediate velocity and enthalpy from the evaluation of the intermediate density $\tilde{\rho}$.

6. INTERMEDIATE DENSITY FOR THE VAN DER WAALS GAS

The linearization procedure outlined in the previous section is now specialized to the case of the polytropic van der Waals gas. The pressure EOS reads

$$P(E,\rho) = \delta\frac{E + a\rho^2}{1 - b\rho} - a\rho^2, \tag{6.1}$$

from which we obtain

$$\frac{\partial P(E,\rho)}{\partial E} = \frac{\delta}{1-b\rho}, \quad \frac{\partial P(E,\rho)}{\partial \rho} = \delta\frac{b(E - a\rho^2) + 2a\rho}{(1-b\rho)^2} - 2a\rho. \tag{6.2}$$

The algebraic form of the van der Waals thermodynamics allows us to obtain the explicit expression of the energy in terms of the two variables (h, ρ) as

$$E(h,\rho) = \frac{(1-b\rho)\rho h - 2a\delta\rho^2}{\delta + 1 - b\rho} + a\rho^2, \tag{6.3}$$

and solve the linearization problem by substituting $E = E(h,\rho)$ in the second part of system (5.8), to obtain

$$\frac{\partial P(E(\tilde{h},\tilde{\rho}),\tilde{\rho})}{\partial E}\Delta E + \frac{\partial P(E(\tilde{h},\tilde{\rho}),\tilde{\rho})}{\partial \rho}\Delta\rho = \Delta P, \tag{6.4}$$

with the understanding $\tilde{h} = \widetilde{h^{\mathrm{t}}} - \frac{\tilde{u}^2}{2}$.

By (6.2) and (6.3), Eq. (6.4) is found to be a third-order polynomial in the intermediate density ratio $r = \tilde{\rho}/\rho c = 3b\tilde{\rho}$, in the form [13],

$$r^3 + Ar^2 + Br + C = 0, \tag{6.5}$$

with coefficients defined in terms of the left and right states as

$$\begin{aligned} A &= \frac{\rho_c}{6P_c}\frac{\Delta P}{\Delta \rho} - 3(2+\delta), \\ B &= \frac{\rho_c}{2P_c}\left[-(2+\delta)\frac{\Delta P}{\Delta \rho} + \delta\left(\frac{\Delta E}{\Delta \rho} - \widetilde{h}^{\mathrm{t}} + \frac{\tilde{u}^2}{2}\right)\right] + 9(1-\delta^2), \\ C &= \frac{3\rho_c}{2P_c}(1+\delta)\left[\frac{\Delta P}{\Delta \rho} - \delta\frac{\Delta E}{\Delta \rho}\right], \end{aligned} \tag{6.6}$$

where ρ_c and P_c are the critical values of the density and pressure, respectively. Therefore, the supplementary equation can be solved analytically by standard formulae. The relevant real root is selected as the one lying within or closer to the interval $[\rho_\ell, \rho_r]$. In the numerical experiments presented in the following section, this simple criterion has been found to be suitable to single out the needed intermediate density.

In the particular case $\Delta\rho = 0$, the supplementary equation (6.4) is linear in $\tilde{\rho}$ and gives

$$r = 3 - 3\delta\frac{\Delta E}{\Delta P}, \tag{6.7}$$

the case $\Delta\rho = 0$ and $\Delta P = 0$ being trivial since one has $\Delta\rho = \Delta P = 0 \Rightarrow \Delta E = 0$ and $\tilde{\rho}$ is therefore arbitrary. We notice that in the limit $b \to 0$ the supplementary equation reduces to a linear equation in $\tilde{\rho}$ whose solution is given by

$$\tilde{\rho} = \frac{\rho_\ell + \rho_r}{2}.$$

7. NUMERICAL RESULTS

The proposed linearization procedure has been applied to the solution of reference shock tube problems for the Euler equations in one spatial dimension. First, we considered a test case proposed in [17] for the water vapor near the liquid–vapor saturation curve. Since in the van der Waals approximation of such a gas $\delta = 0.329 > \delta^*$, the fundamental derivative $\mathcal{G}$ is always positive outside the two-phase region, and no anomalous behavior is observed in the vapor phase. In the considered numerical experiment, the diaphragm is located at $x = 0.5$ and separates the following constant initial states, made dimensionless by critical values:

	ρ_ℓ	u_ℓ	P_ℓ	$\mathcal{G}_\ell$	ρ_r	u_r	P_r	$\mathcal{G}_r$
WV1	1.01000	0	1.60770	2.23946	0.59400	0	0.89570	1.36136

In Fig. 3, numerical solution of case WV1 is compared with the one obtained by the Davis method [9], which has been used, for example, by Argrow [2] for the computation of the nonclassical behavior of the van der Waals gas. The computations have been performed over a 400-point grid by means of a high-resolution flux-limiter method, which takes advantage of the proposed linearization near discontinuities and uses a Lax–Wendroff scheme in smooth flow regions; see, for instance, LeVeque [18]. Results are very similar to those of

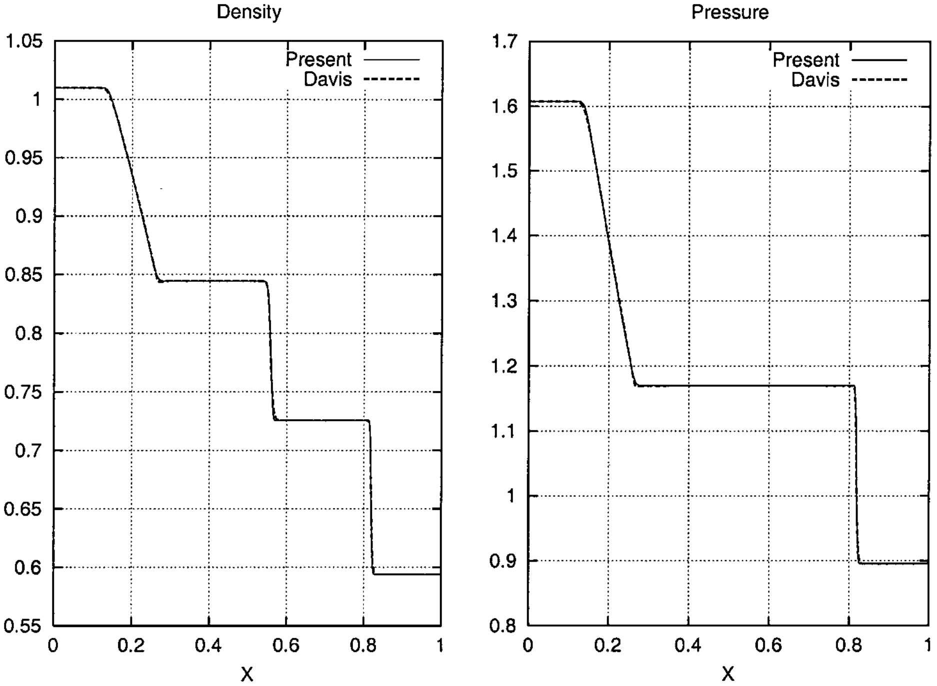

FIG. 3. Numerical solution of the Riemann problem for test case WV1. Solution at the dimensionless time $t^* = (t/L)(P_c/\rho_c)^{1/2} = 0.2$, $\Delta t^* = 1 \times 10^{-3}$.

the Davis method, although the present method achieves a slightly better resolution of the wave structure as can be appreciated in the enlargements of Fig. 4.

In Figs. 5–8 numerical results including nonclassical phenomena are reported. These shock tube problems have been proposed by Argrow [2] to explore the nonclassical behavior

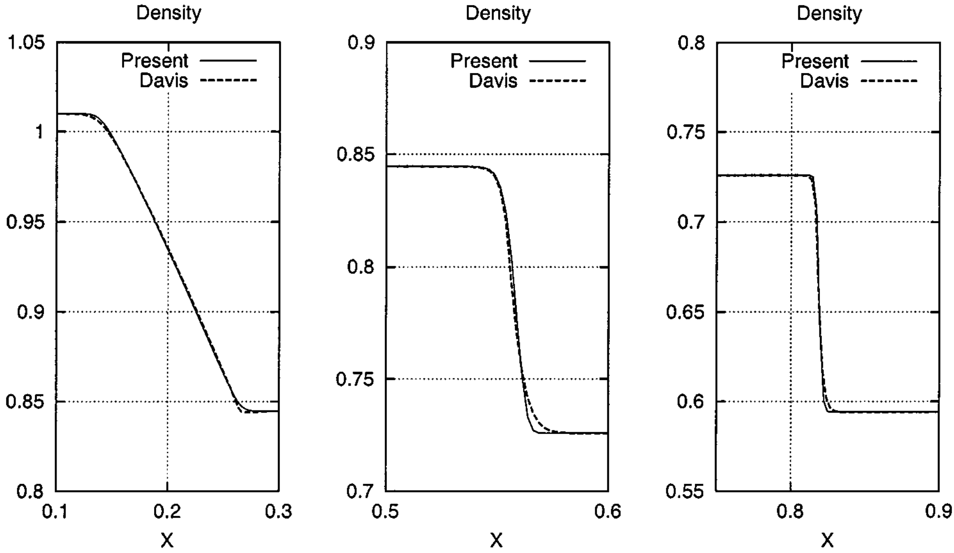

FIG. 4. Enlargement of the density distribution for case WV1. Left: rarefaction wave. Center: contact discontinuity. Right: shock wave.

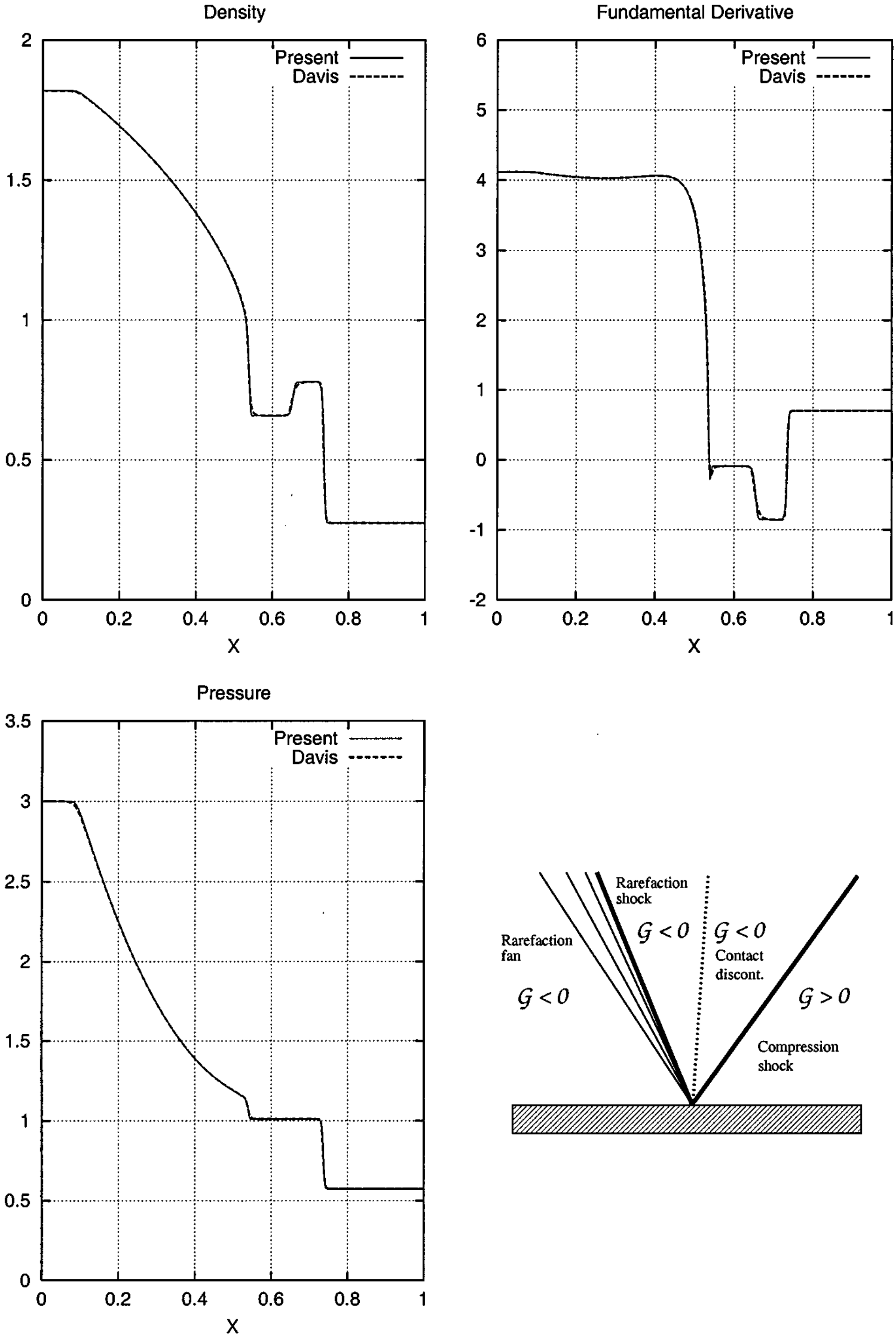

FIG. 5. Numerical solution of the Riemann problem for test case DG1. Solution at the dimensionless time $t^* = 0.15$, $\Delta t^* = 5 \times 10^{-4}$.

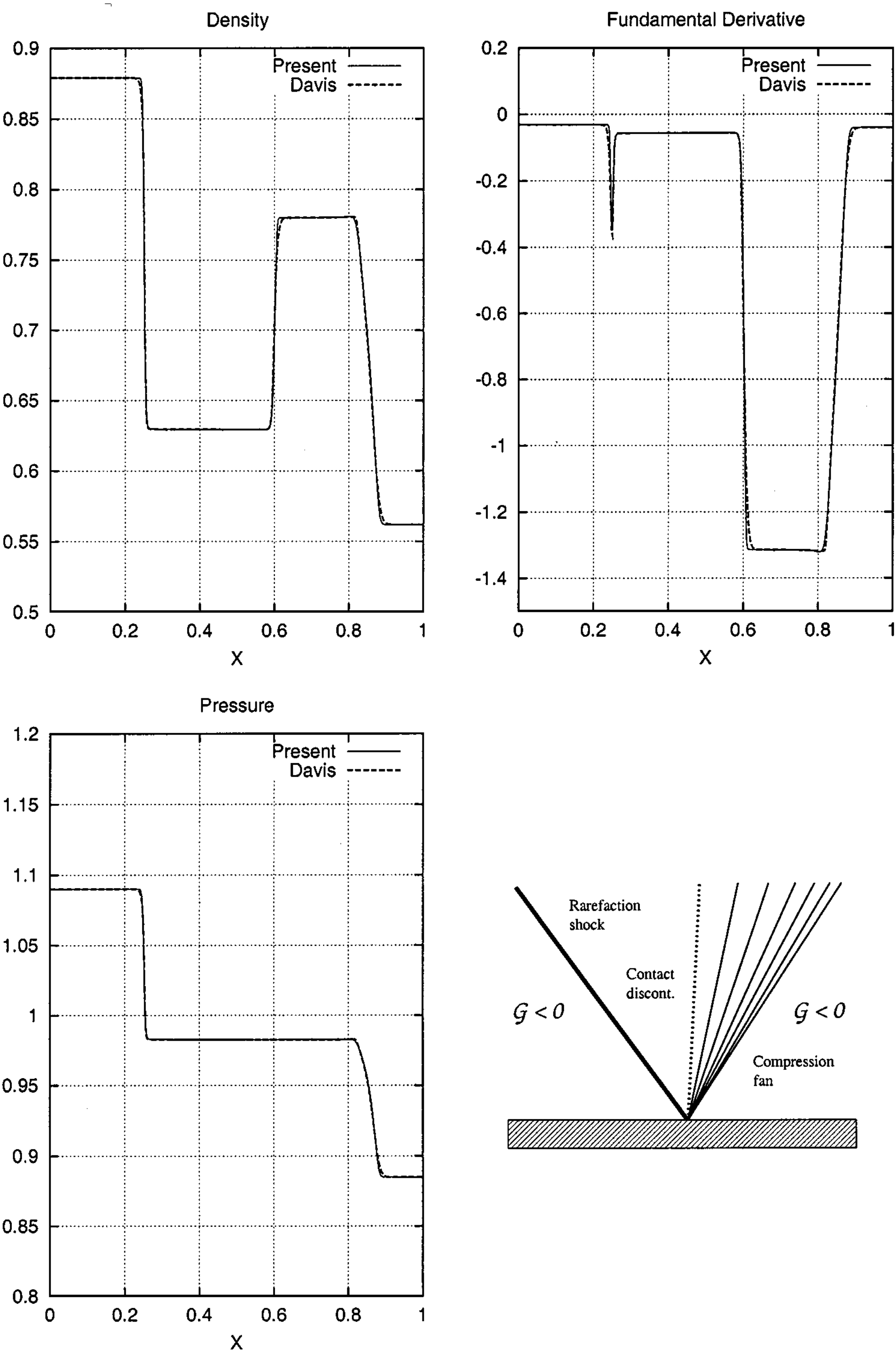

FIG. 6. Numerical solution of the Riemann problem for test case DG2. Solution at the dimensionless time $t^* = 0.45$, $\Delta t^* = 1.5 \times 10^{-3}$.

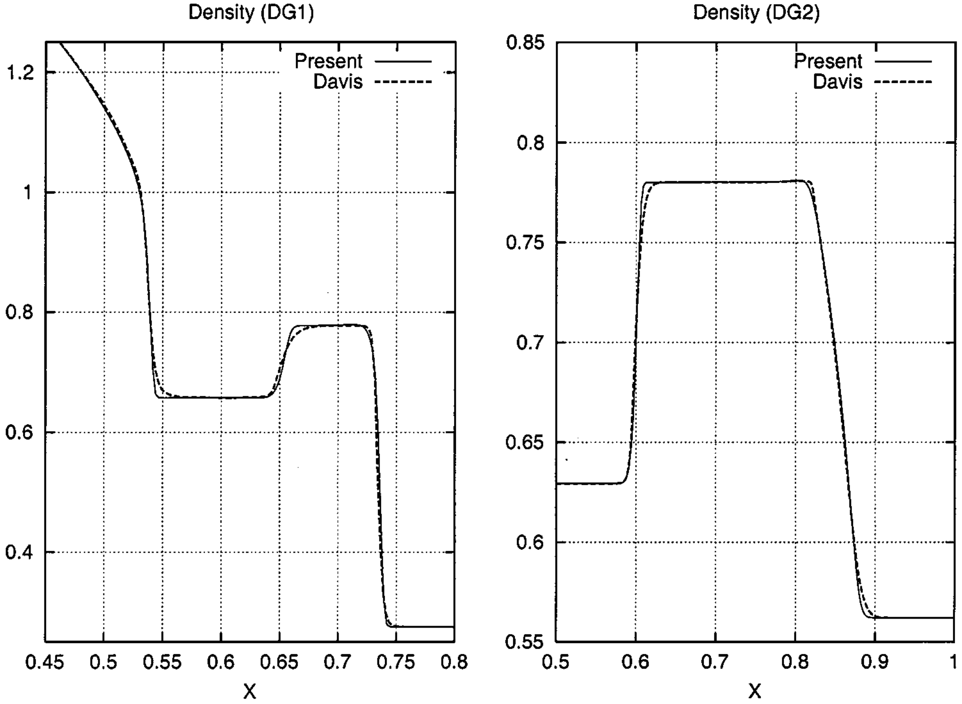

FIG. 7. Comparison of the proposed method and the method of Davis for the resolution of cases DG1 and DG2.

of a van der Waals gas near the critical point, and are defined by the following dimensionless quantities:

	ρ_ℓ	u_ℓ	P_ℓ	$\mathcal{G}_\ell$	ρ_r	u_r	P_r	$\mathcal{G}_r$
DG1	1.818	0	3.000	4.118	0.275	0	0.575	0.703
DG2	0.879	0	1.090	−0.031	0.562	0	0.885	−4.016
DG3	0.879	0	1.090	−0.031	0.275	0	0.575	0.703.

The numerical results are computed on a 400-point grid with $\delta = 0.0125$, which corresponds to a fluid with a large specific heat with respect to its molecular weight as, for instance, PP10, $C_{13}F_{22}$ ($\delta = 0.0128$).

The DG1 case corresponds to the situation exemplified in Fig. 2, where the initial gas states belong to the $\mathcal{G} > 0$ region but the $\mathcal{G} = 0$ boundary in the v-P plane is crossed during the flow evolution. A mixed rarefaction wave is formed, composed by a transonic rarefaction fan connected to a rarefaction shock propagating to the right. This rarefaction shock occurs when the $\mathcal{G}$ values become negative. On the other hand, the compression shock propagating toward the low pressure side satisfies the Rankine–Hugoniot conditions, and it is therefore a classical shock even if it connects two states with different sign of $\mathcal{G}$. This indicates that the crossing of the $\mathcal{G} = 0$ boundary cannot be taken as a sufficient condition for the existence of mixed waves.

The DG2 case is a typical example of nonclassical behavior, since the initial gas states belong entirely to the nonconvex region and moreover the fundamental derivative remains negative in the whole flow field during the flow evolution. A rarefaction shock and a continuous compression fan are observed in Fig. 6.

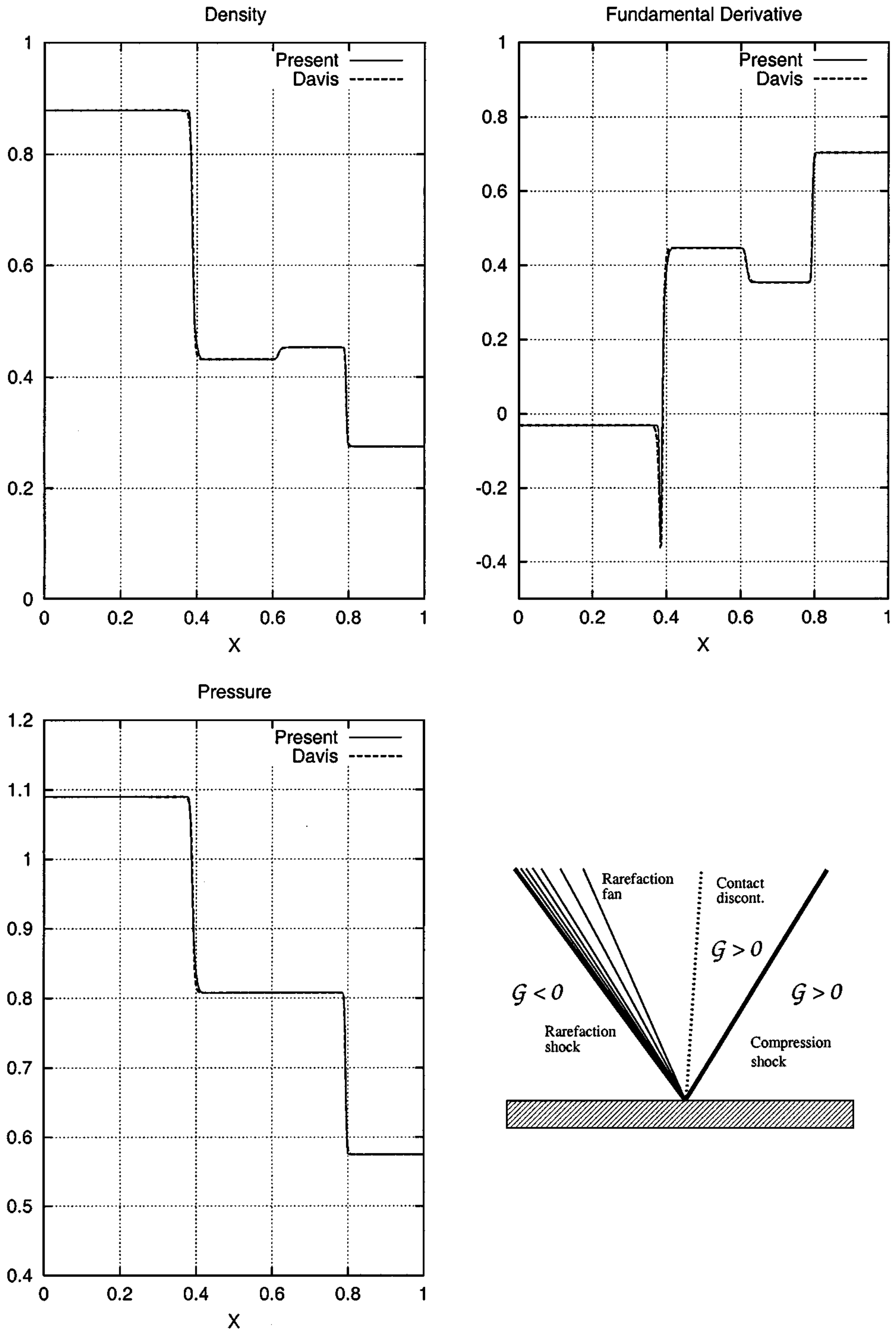

FIG. 8. Numerical solution of the Riemann problem for test case DG3. Solution at the dimensionless time $t^* = 0.2$, $\Delta t^* = 1 \times 10^{-3}$.

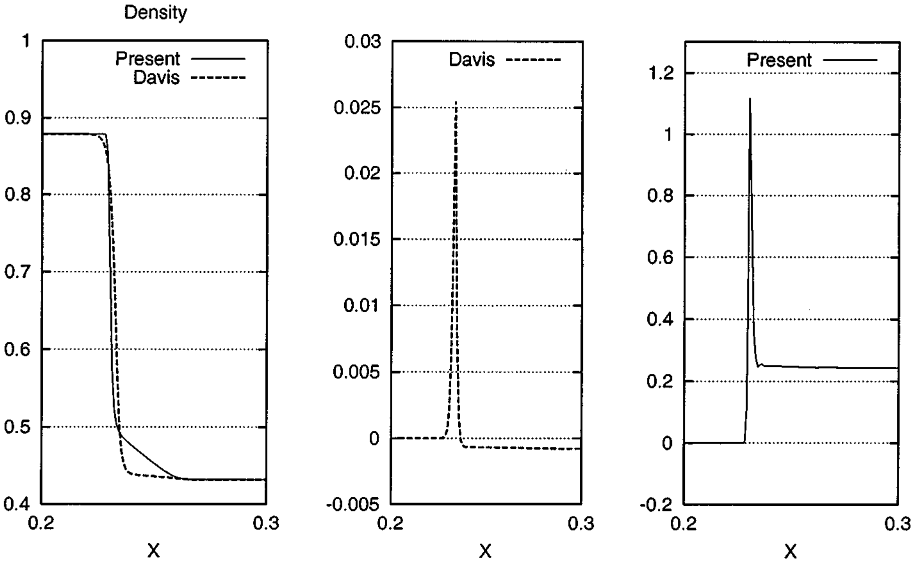

FIG. 9. Mixed rarefaction wave of case DG3 at time $t^* = 0.48$ on a 1000-node grid. Density profile (right) and entropy difference ×1000 (center and right). The entropy difference is defined as $s(T, v)/s(T_\ell, v_\ell) - 1$.

The comparison with Davis method yields very similar results also for the DG1 and DG2 cases. Differences may be appreciated only locally on the wave resolution (Fig. 7). As expected, the proposed upwind scheme behaves better than the artificial viscosity scheme in capturing contact discontinuities, which appear sharper using the proposed approach. The above becomes more evident by reducing the spatial resolution.

The last test case, DG3 (Fig. 8), presents however a subtle but important difference between Davis and present results. This case has an initial left, high pressure state lying in the $\mathcal{G} < 0$ region, while the right state is well within the convex region. The gas expansion starts as a rarefaction shock that turns into a small rarefaction fan once the $\mathcal{G} = 0$ boundary is crossed. In Fig. 9, an enlargement of the mixed wave as computed by the Davis scheme and the present scheme is shown. The difference in the density profile can be explained by examining the entropy production through the rarefaction shock. The Davis scheme computes a negative (nonphysical) entropy difference, while the present scheme is found to satisfy the entropy condition. As a result, the isentropic rarefaction fan occurs along different isentropes for the two schemes, thus leading to different density profiles. Moreover, for the same reason, the speed of the rarefaction shock as computed by the present scheme is higher than the one obtained from the Davis scheme.

Comparisons with other standard extensions of Roe scheme and, in particular, with the one proposed in [33] showed almost no differences with present results. It could be possible that a different behavior between the present method and other extended Roe schemes may be found in the simulation of flow fields that include phase transition. In fact, as pointed out in [31], Roe linearizations based on the quasi-Jacobian form may break down in the two-phase region due to inconsistency among intermediate thermodynamic quantities.

As a final remark, we notice that LeVeque's entropy fix [18], originally considered in the present scheme, has been found to fail in the presence of a negative/positive transonic

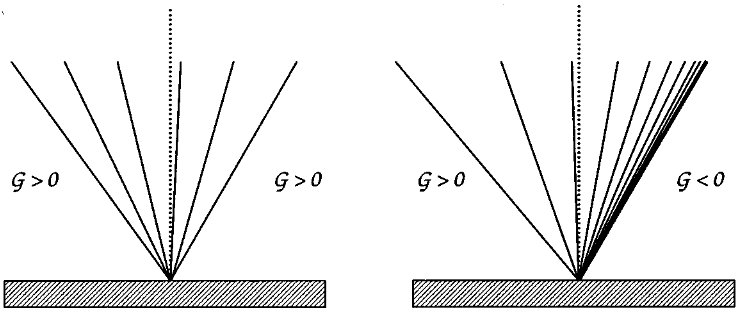

FIG. 10. Density contours in the kinematic plane (x, t) for classical (left) and nonclassical transonic rarefaction.

rarefaction (case DG1). This difficulty is caused by the nonclassical character of the rarefaction waves in that Riemann problem (see Fig. 10), which is extraneous to LeVeque's entropy fix developed for classical transonic rarefactions. The difficulty has been easily circumvented by replacing LeVeque's entropy fix with the standard entropy fix of Harten and Hyman [15].

8. CONCLUSIONS

In the present work, the linearization procedure of Roe for the Euler equations has been extended from the ideal gas to a gas governed by the van der Waals equations of state. The proposed method assumes an intermediate state as the unknown of the linearization problem and, differently from standard procedures for the ideal gas, requires the determination of an *intermediate density* in addition to the intermediate velocity and total enthalpy of the original method of Roe. Such a density is needed to evaluate the eigenstructure of the Jacobian matrix, due to the nonideal form of the equations of state employed. The choice of the Jacobian form ensures the automatic satisfaction of the consistency and hyperbolicity properties of the scheme. Pressure derivatives with respect to the conservative variables appearing in the Roe (Jacobian) matrix are not assumed to be additional unknowns, but are merely considered as functions of the intermediate state given by the variables density, velocity, and total specific enthalpy. The originality of the proposed method lies in the introduction of a convenient supplementary condition which decouples the determination of the intermediate velocity and enthalpy—given by the standard Roe average—from the determination of the intermediate density. Thanks to the analytical form of the van der Waals thermodynamics, a third-order algebraic equation for the intermediate density is obtained, which directly gives the solution of the linearization problem in terms of the Roe averaged velocity and total enthalpy and of the jumps in the density, pressure, and internal energy per unit volume.

By virtue of the segregation of all the aspects dependent on the thermodynamic equations of state into a single equation for the intermediate density, the present method can be easily extended to deal with more complex physical systems such as, for instance, accurate thermodynamic models for dense gases or chemically reacting gases in local thermodynamic equilibrium.

APPENDIX A: SOLUTION OF THE LINEARIZATION PROBLEM

In this appendix, following [14], system (5.4) is derived from (5.2) by augmenting it with the supplementary equation (5.3). Particular cases in which the outlined solution breaks down due to the division of vanishing quantities are dealt with in the next section.

Let us first rewrite system (5.2), namely,

$$\begin{cases} (\Delta\rho)\left(\dfrac{\tilde{m}}{\tilde{\rho}}\right)^2 - 2(\Delta m)\dfrac{\tilde{m}}{\tilde{\rho}} + \Delta\left(\dfrac{m^2}{\rho}\right) + (\Delta P - \nabla_{\boldsymbol{w}}\Pi(\tilde{\boldsymbol{w}})\cdot\Delta\boldsymbol{w}) = 0, \\ -(\Delta\rho)\dfrac{\tilde{m}}{\tilde{\rho}}\dfrac{\widetilde{E^{\mathrm{t}}}+\Pi(\tilde{\boldsymbol{w}})}{\tilde{\rho}} + (\Delta m)\dfrac{\widetilde{E^{\mathrm{t}}}+\Pi(\tilde{\boldsymbol{w}})}{\tilde{\rho}} + (\Delta E^{\mathrm{t}})\dfrac{\tilde{m}}{\tilde{\rho}} + \dfrac{\tilde{m}}{\tilde{\rho}}\nabla_{\boldsymbol{w}}\Pi(\tilde{\boldsymbol{w}})\cdot\Delta\boldsymbol{w} \\ \qquad = \Delta\left(\dfrac{m}{\rho}(E^{\mathrm{t}}+\Pi)\right), \end{cases} \tag{A.1}$$

in a more convenient form. We now suppose that $\Delta\rho = \rho_r - \rho_\ell$ and $\Delta m = m_r - m_\ell$ are both different from zero; the particular cases of data for the Riemann problem not fulfilling these conditions will be dealt with separately later on. Then, provided that

$$\Delta m - \frac{\tilde{m}}{\tilde{\rho}}\Delta\rho \neq 0, \tag{A.2}$$

the one-parameter family of solutions is obtained from the following system

$$\begin{cases} \dfrac{\tilde{m}}{\tilde{\rho}} = \dfrac{1}{\Delta\rho}\left\{\Delta m \pm \sqrt{(\Delta m)^2 - (\Delta\rho)\left[\Delta\left(\dfrac{m^2}{\rho}\right) + (\Delta P - \nabla_{\boldsymbol{w}}\Pi(\tilde{\boldsymbol{w}})\cdot\Delta\boldsymbol{w})\right]}\,\right\}, \\ \dfrac{\widetilde{E^{\mathrm{t}}}+\Pi(\tilde{\boldsymbol{w}})}{\tilde{\rho}} = \left(\Delta m - \dfrac{\tilde{m}}{\tilde{\rho}}\Delta\rho\right)^{-1}\left[\Delta\left(\dfrac{m}{\rho}(E^{\mathrm{t}}+\Pi)\right) - \dfrac{\tilde{m}}{\tilde{\rho}}(\Delta E^{\mathrm{t}} + \nabla_{\boldsymbol{w}}\Pi(\tilde{\boldsymbol{w}})\cdot\Delta\boldsymbol{w})\right], \end{cases} \tag{A.3}$$

where the first equation has been rewritten by exploiting the quadratic solution formula. This is a system of two coupled equations in the three unknowns $(\tilde{\rho}, \tilde{m}, \widetilde{E^{\mathrm{t}}})^{\mathrm{T}} = \tilde{\boldsymbol{w}}$. We notice that the coupling is due to the presence of the unknown $\tilde{\boldsymbol{w}}$ in the function $\Pi(\tilde{\boldsymbol{w}})$ on the left-hand side of the second equation, and to the presence of the ratio $\tilde{m}/\tilde{\rho}$ and of the gradient $\nabla_{\boldsymbol{w}}\Pi(\tilde{\boldsymbol{w}})$ on the right-hand sides.

We now substitute the supplementary equation (5.3), namely,

$$\nabla_{\boldsymbol{w}}\Pi(\tilde{\boldsymbol{w}})\cdot\Delta\boldsymbol{w} = \Delta P, \tag{A.4}$$

into the above system, so that the first equation of system (A.3) can now be written so as to express the ratio $\tilde{m}/\tilde{\rho}$ as

$$\frac{\tilde{m}}{\tilde{\rho}} = \frac{1}{\Delta\rho}\left[\Delta m \pm \sqrt{(\Delta m)^2 - (\Delta\rho)\Delta\left(\frac{m^2}{\rho}\right)}\,\right]. \tag{A.5}$$

The equation above has two different solutions and hence we have to choose the physically relevant one. Let us first consider the discriminant in (A.5). By substituting the variations $\Delta m = m_r - m_\ell$ and $\Delta\rho = \rho_r - \rho_\ell$, the condition for a positive discriminant reads

$$m_r^2 - 2m_r m_\ell + m_\ell^2 - (\rho_r - \rho_\ell)\left(\frac{m_r^2}{\rho_r} - \frac{m_\ell^2}{\rho_\ell}\right) \geq 0,$$

that can be written as the ratio of two quantities

$$\frac{(\rho_\ell m_r - \rho_r m_\ell)^2}{\rho_\ell \rho_r} \geq 0. \tag{A.6}$$

The denominator is always positive whereas the numerator is only nonnegative. Therefore, Eq. (A.5) has two real distinct solutions except when

$$\frac{m_\ell}{\rho_\ell} = \frac{m_r}{\rho_r},$$

in which case the root is double. This special situation, which was excluded by imposing condition (A.2), corresponds to a constant velocity across the left and right states and will be dealt with in the following.

Considering now a positive discriminant, the solution of the quadratic equation (A.5) for the ratio $\tilde{m}/\tilde{\rho}$ may be written as

$$\frac{\tilde{m}}{\tilde{\rho}} = \frac{1}{\rho_r - \rho_\ell}\left\{m_r - m_\ell \pm \frac{\rho_\ell m_r - \rho_r m_\ell}{\sqrt{\rho_\ell \rho_r}}\right\}. \tag{A.7}$$

The solution obtained by taking the negative sign in the expression reads

$$\frac{\tilde{m}}{\tilde{\rho}} = \frac{\frac{m_\ell}{\sqrt{\rho_\ell}} + \frac{m_r}{\sqrt{\rho_r}}}{\sqrt{\rho_\ell} + \sqrt{\rho_r}}, \tag{A.8}$$

whereas, by taking the positive sign in (A.7), we have

$$\frac{\tilde{m}}{\tilde{\rho}} = \frac{\frac{m_\ell}{\sqrt{\rho_\ell}} - \frac{m_r}{\sqrt{\rho_r}}}{\sqrt{\rho_\ell} - \sqrt{\rho_r}}.$$

This result is rejected since it leads to an infinite value for the ratio $\tilde{m}/\tilde{\rho}$ when $\Delta\rho \to 0$, if m_ℓ and m_r are fixed.

The resulting system of three equations now reads

$$\begin{cases} \nabla_{\boldsymbol{w}} \Pi(\tilde{\boldsymbol{w}}) \cdot \Delta \boldsymbol{w} = \Delta P, \\ \dfrac{\tilde{m}}{\tilde{\rho}} = \dfrac{\frac{m_\ell}{\sqrt{\rho_\ell}} + \frac{m_r}{\sqrt{\rho_r}}}{\sqrt{\rho_\ell} + \sqrt{\rho_r}}, \\ \dfrac{\widetilde{E^{\mathrm{t}}} + \Pi(\tilde{\boldsymbol{w}})}{\tilde{\rho}} = \dfrac{\Delta\left(\frac{m}{\rho}(E^{\mathrm{t}} + \Pi)\right) - \frac{\tilde{m}}{\tilde{\rho}}\Delta(E^{\mathrm{t}} + \Pi)}{\Delta m - \frac{\tilde{m}}{\tilde{\rho}}\Delta\rho}. \end{cases}$$

By rewriting the last term in the right-hand side of the energy equation in the slightly different form,

$$\frac{\widetilde{E^{\mathrm{t}}} + \Pi(\tilde{w})}{\tilde{\rho}} = \frac{\Delta\left(m\frac{E^{\mathrm{t}}+\Pi}{\rho}\right) - \frac{\tilde{m}}{\tilde{\rho}}\Delta\left(\rho\frac{E^{\mathrm{t}}+\Pi}{\rho}\right)}{\Delta m - \frac{\tilde{m}}{\tilde{\rho}}\Delta\rho},$$

and by substituting the value of $\tilde{m}/\tilde{\rho}$ given by (A.8) into the equation above we obtain the system

$$\begin{aligned} \nabla_w \Pi(\tilde{w}) \cdot \Delta w &= \Delta P, \\ \frac{\tilde{m}}{\tilde{\rho}} &= \frac{\frac{m_\ell}{\sqrt{\rho_\ell}} + \frac{m_r}{\sqrt{\rho_r}}}{\sqrt{\rho_\ell} + \sqrt{\rho_r}}, \\ \frac{\widetilde{E^{\mathrm{t}}} + \Pi(\tilde{w})}{\tilde{\rho}} &= \frac{\frac{E^{\mathrm{t}}_\ell + \Pi(w_\ell)}{\sqrt{\rho_\ell}} + \frac{E^{\mathrm{t}}_r + \Pi(w_r)}{\sqrt{\rho_r}}}{\sqrt{\rho_\ell} + \sqrt{\rho_r}}, \end{aligned} \tag{A.9}$$

that is, system (5.4).

APPENDIX B: SPECIAL CASES OF ROE LINEARIZATION FOR NONIDEAL GASES

The solution of the linearization problem for the Euler equations described above may break down due to the division by vanishing quantities. This occurs either when the density is the same in the left and right states or when the term $\Delta m - \frac{\tilde{m}}{\tilde{\rho}}\Delta\rho$ is equal to zero. The particular case $\Delta\rho = \Delta E = 0$ is trivial since thermodynamics implies $\Delta P = 0$ and therefore, being the supplementary equation an identity, the intermediate density is arbitrary, the other two variables being recovered as solutions of the second and third equations of system (A.9).

B.1. The Case $\Delta\rho = 0$, $\Delta m \neq 0$

If $\Delta\rho = 0$, that is, $\rho_\ell = \rho_r = \rho_{\ell r}$, the linearization problem consisting of system (A.1) augmented with the supplementary equation (A.4) simplifies to

$$\begin{cases} \Pi_m(\tilde{\boldsymbol{w}})\Delta m + \Pi_{E^{\mathrm{t}}}(\tilde{\boldsymbol{w}})\Delta E^{\mathrm{t}} = \Delta P, \\ \left[\dfrac{2\tilde{m}}{\tilde{\rho}} + \Pi_m(\tilde{\boldsymbol{w}})\right]\Delta m + \Pi_{E^{\mathrm{t}}}(\tilde{\boldsymbol{w}})\Delta E^{\mathrm{t}} = \Delta\left(\dfrac{m^2}{\rho} + \Pi\right), \\ \left[\dfrac{1}{\tilde{\rho}}\left(\widetilde{E^{\mathrm{t}}} + \Pi(\tilde{\boldsymbol{w}})\right) + \dfrac{\tilde{m}}{\tilde{\rho}}\Pi_m(\tilde{\boldsymbol{w}})\right]\Delta m + \dfrac{\tilde{m}}{\tilde{\rho}}(1 + \Pi_{E^{\mathrm{t}}}(\tilde{\boldsymbol{w}}))\Delta E^{\mathrm{t}} = \Delta\left(\dfrac{m}{\rho}(E^{\mathrm{t}} + \Pi)\right). \end{cases} \tag{B.1}$$

The first and the second equations give

$$\frac{2\tilde{m}}{\tilde{\rho}}\Delta m = \Delta\left(\frac{m^2}{\rho}\right) \longrightarrow \frac{\tilde{m}}{\tilde{\rho}} = \frac{m_\ell + m_r}{2\rho_{\ell r}}.$$

By substituting the ratio $\tilde{m}/\tilde{\rho}$ into the third equation of (B.1) we obtain

$$\frac{\widetilde{E^{\mathrm{t}}} + \Pi(\tilde{\boldsymbol{w}})}{\tilde{\rho}}\Delta m = \frac{E^{\mathrm{t}}_\ell + \Pi(\boldsymbol{w}_\ell) + E^{\mathrm{t}}_r + \Pi(\boldsymbol{w}_r)}{2\rho_{\ell r}}\Delta m.$$

Therefore, if $\Delta m \neq 0$, the system becomes

$$\begin{cases} \Pi_m(\tilde{w})\Delta m + \Pi_{E^{\mathrm{t}}}(\tilde{w})\Delta E^{\mathrm{t}} = \Delta P, \\[2mm] \dfrac{\tilde{m}}{\tilde{\rho}} = \dfrac{m_\ell + m_r}{2\rho_{\ell r}}, \\[2mm] \dfrac{\widetilde{E^{\mathrm{t}}} + \Pi(\tilde{w})}{\tilde{\rho}} = \dfrac{E^{\mathrm{t}}_\ell + \Pi(w_\ell) + E^{\mathrm{t}}_r + \Pi(w_r)}{2\rho_{\ell r}}. \end{cases}$$

Introducing now the change of variable $w = (\rho, m, E^{\mathrm{t}}) \to v = (\rho, u, h^{\mathrm{t}})$, we obtain

$$\begin{cases} \tilde{u} = \dfrac{u_\ell + u_r}{2}, \quad \widetilde{h^{\mathrm{t}}} = \dfrac{h^{\mathrm{t}}_\ell + h^{\mathrm{t}}_r}{2}, \\[2mm] \begin{cases} \dfrac{\partial P(\tilde{E}, \tilde{\rho})}{\partial E}\Delta E = \Delta P, \\[2mm] \dfrac{\tilde{E} + P(\tilde{E}, \tilde{\rho})}{\tilde{\rho}} = \widetilde{h^{\mathrm{t}}} - \dfrac{\tilde{u}^2}{2}, \end{cases} \end{cases} \tag{B.2}$$

where the relation for the energy $\tilde{E}$ has been written to close the system. We notice that, although $\rho_\ell = \rho_r = \rho_{\ell r}$, the intermediate density $\tilde{\rho}$, solution of the supplementary equation, is in general different from $\rho_{\ell r}$.

B.2. The Case $\Delta\rho = 0$, $\Delta m = 0$

In the very particular case $\Delta\rho = 0$ and $\Delta m = 0$, the linearization problem simplifies further to

$$\begin{cases} \Pi_{E^{\mathrm{t}}}(\tilde{\boldsymbol{w}})\Delta E^{\mathrm{t}} = \Delta P, \\[2mm] \Pi_{E^{\mathrm{t}}}(\tilde{\boldsymbol{w}})\Delta E^{\mathrm{t}} = \Delta P, \\[2mm] \dfrac{\tilde{m}}{\tilde{\rho}}(1 + \Pi_{E^{\mathrm{t}}}(\tilde{\boldsymbol{w}}))\Delta E^{\mathrm{t}} = \dfrac{m_{\ell r}}{\rho_{\ell r}}\Delta(E^{\mathrm{t}} + \Pi), \end{cases} \tag{B.3}$$

that is, the supplementary equation and the equation stemming from the conservation of momentum are the same. Eliminating the quantity $\Pi_{E^{\mathrm{t}}}(\tilde{w})\Delta E^{\mathrm{t}}$ in the last equation, we obtain the single relation

$$\frac{\tilde{m}}{\tilde{\rho}}\Delta(E^{\mathrm{t}} + \Pi) = \frac{m_{\ell r}}{\rho_{\ell r}}\Delta(E^{\mathrm{t}} + \Pi),$$

which gives immediately

$$\frac{\tilde{m}}{\tilde{\rho}} = \frac{m_{\ell r}}{\rho_{\ell r}},$$

since $\Delta(E^{\mathrm{t}} + \Pi) \neq 0$. Therefore, in this particular case the intermediate state $\tilde{w}$ is the solution of the system

$$\begin{cases} \Pi_{E^{\mathrm{t}}}(\tilde{\boldsymbol{w}}) = \dfrac{\Delta P}{\Delta E^{\mathrm{t}}}, \\[2mm] \dfrac{\tilde{m}}{\tilde{\rho}} = \dfrac{m_{\ell r}}{\rho_{\ell r}}, \end{cases} \tag{B.4}$$

which has a one-parameter family of solutions. As remarked, in this very special case, the momentum equation is coincident with the one resulting from the auxiliary condition

$$\nabla_w \Pi(\tilde{w}) \cdot \Delta w = \Delta P,$$

introduced eventually to select a unique intermediate state and hence an additional condition is to be given to define both the intermediate state $\tilde{w}$ and the Roe matrix completely. Introducing now the change of variable $w = (\rho, m, E^{\mathrm{t}}) \to v = (\rho, u, h^{\mathrm{t}})$, and fixing the available parameter by selecting the standard average of the enthalpy, namely,

$$\widetilde{h^{\mathrm{t}}} = \frac{\sqrt{\rho_\ell}\, h^{\mathrm{t}}_\ell + \sqrt{\rho_r}\, h^{\mathrm{t}}_r}{\sqrt{\rho_\ell} + \sqrt{\rho_r}} = \frac{h^{\mathrm{t}}_\ell + h^{\mathrm{t}}_r}{2},$$

we have

$$\begin{cases} \tilde{u} = \dfrac{u_\ell + u_r}{2}, \quad \widetilde{h^{\mathrm{t}}} = \dfrac{h^{\mathrm{t}}_\ell + h^{\mathrm{t}}_r}{2}, \\ \begin{cases} \frac{\partial P(\tilde{E}, \tilde{\rho})}{\partial E} \Delta E = \Delta P, \\ \frac{\tilde{E} + P(\tilde{E}, \tilde{\rho})}{\tilde{\rho}} = \widetilde{h^{\mathrm{t}}} - \frac{\tilde{u}^2}{2}, \end{cases} \end{cases} \tag{B.5}$$

where again the relation for the energy $\tilde{E}$ has been written to close the system. To conclude, we notice that, due to the particular choice for the average total enthalpy, the intermediate state obtained in this special case has the same form as in the previous section.

B.3. The Case $\Delta m = \frac{\tilde{m}}{\tilde{\rho}} \Delta\rho$, $\Delta\rho \neq 0$, $\Delta m \neq 0$

We now go back to considering the situation associated with the breakdown in the solution of the energy equation in (5.4), namely the condition

$$\Delta m - \frac{\tilde{m}}{\tilde{\rho}} \Delta\rho = 0. \tag{B.6}$$

In the following, one can assume $\Delta\rho \neq 0$ since the very special case $\Delta\rho = \Delta m = 0$ has been already considered in the previous section.

The condition $\Delta m = \frac{\tilde{m}}{\tilde{\rho}} \Delta\rho$ corresponds to the vanishing of the square root in Eq. (A.5) so the intermediate state is defined by the following set of three equations easily recovered from the general system (A.1)

$$\begin{cases} \boldsymbol{\nabla}_w \Pi(\tilde{w}) \cdot \Delta w = \Delta P, \\ \dfrac{\tilde{m}}{\tilde{\rho}} = \dfrac{\Delta m}{\Delta \rho}, \\ \dfrac{\tilde{m}}{\tilde{\rho}} \Delta(E^{\mathrm{t}} + \Pi) = \Delta\left(\dfrac{m}{\rho}(E^{\mathrm{t}} + \Pi)\right). \end{cases} \tag{B.7}$$

By eliminating $\tilde{m}/\tilde{\rho}$ from the second and the third equation we obtain the relation

$$\frac{\Delta m}{\Delta \rho} \Delta(E^{\mathrm{t}} + \Pi) = \Delta\left(\frac{m}{\rho}(E^{\mathrm{t}} + \Pi)\right),$$

in which no unknown appears and that must therefore be an identity for the system to be solvable. By evaluating the variations appearing in the relation above we have

$$\frac{m_r - m_\ell}{\rho_r - \rho_\ell}\big(E_r^{\mathrm{t}} - E_\ell^{\mathrm{t}} + \Pi(\boldsymbol{w}_r) - \Pi(\boldsymbol{w}_\ell)\big) = \frac{m_r}{\rho_r}\big(E_r^{\mathrm{t}} + \Pi(\boldsymbol{w}_r)\big) - \frac{m_\ell}{\rho_\ell}\big(E_\ell^{\mathrm{t}} + \Pi(\boldsymbol{w}_\ell)\big),$$

which is a trivial identity for any pressure function $\Pi(w)$ if one can show that

$$\frac{m_r - m_\ell}{\rho_r - \rho_\ell} = \frac{m_r}{\rho_r} \quad \text{and} \quad \frac{m_r - m_\ell}{\rho_r - \rho_\ell} = \frac{m_\ell}{\rho_\ell}.$$

These two relations are satisfied identically provided that

$$\frac{m_\ell}{\rho_\ell} = \frac{m_r}{\rho_r},$$

which is indeed the case we are considering.

Therefore, in the case $m_\ell/\rho_\ell = m_r/\rho_r$, the third equation is identically satisfied and the problem simplifies to

$$\begin{cases} \boldsymbol{\nabla}_w \Pi(\tilde{\boldsymbol{w}}) \cdot \Delta \boldsymbol{w} = \Delta P, \\ \dfrac{\tilde{m}}{\tilde{\rho}} = \dfrac{\Delta m}{\Delta \rho}, \end{cases} \tag{B.8}$$

so that there is a one-parameter family of solutions and therefore an additional condition should be imposed in this case to determine the intermediate state completely. If we again consider the change of variable $w = (\rho, m, E^{\mathrm{t}}) \to v = (\rho, u, h^{\mathrm{t}})$, and fix the available parameter by selecting the arithmetic average of the enthalpy, we have

$$\begin{cases} \tilde{u} = u_{\ell r}, \quad \widetilde{h^{\mathrm{t}}} = \dfrac{h_\ell^{\mathrm{t}} + h_r^{\mathrm{t}}}{2}, \\ \begin{cases} \dfrac{\partial P(\tilde{E}, \tilde{\rho})}{\partial E} \Delta E + \dfrac{\partial P(\tilde{E}, \tilde{\rho})}{\partial \rho} \Delta \rho = \Delta P, \\ \dfrac{\tilde{E} + P(\tilde{E}, \tilde{\rho})}{\tilde{\rho}} = \widetilde{h^{\mathrm{t}}} - \dfrac{\tilde{u}^2}{2}. \end{cases} \end{cases} \tag{B.9}$$

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