Numerical schemes for quasi-1D steady nozzle flows

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Abstract

In this work we construct high-resolution numerical schemes for the calculation of the quasi-1D unsteady flow in pipes with variable cross-sectional area. This is an example of non-homogeneous hyperbolic systems of conservation laws that admit stationary solutions. We use the strategy developed by the authors in [1] which is to transform the non-homogeneous system into homogeneous writing the source term in divergence form, so that it can be incorporated into the flux vector of the homogeneous system and discretized in the same way. As a result, the source terms are automatically discretized to achieve perfect balance with flux terms, obtaining well-balanced schemes that produce very robust and accurate solutions. Concretely, the mentioned strategy will be used to extend the flux limiter technique [2] and the Harten, Lax and van Leer (HLL) Riemann solver [3] to the quasi-1D flow in ducts of variable cross-section. The numerical results confirm the capacity of these methods to construct well-balanced schemes.

Keywords: conservation law; source term; well-balanced scheme

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1. Introduction

The main difficulty in solving numerically hyperbolic systems of conservation laws is the necessity to accurately reproduce the discontinuities that can arise in the solution even when initial data is smooth. Basic high-resolution techniques for the integration of such problems have been developed during the last decades (see, for example, [2],[3], [4], [5] and [6]). These techniques are characterized by being higher-order in smooth regions of the solution, preventing the presence of false numerical oscillations which appear with the use of the classical second-order schemes around the discontinuities. More recently attention has been turning towards the study of hyperbolic systems of conservation laws with source terms because of these systems govern many problems of practical interest (see, for exemple, [1],[7], [8], [9], [10], [11] and [12]). In the non-homogeneous case, the development of these techniques gives the difficulty added by the presence of the source terms that need a different treatment depending, most of the times, on the physical problem that they model.

Special attention requires the numerical treatment when non-homogeneous hyperbolic systems admit steady solutions. In particular, many of the problems that appear to approximate numerically solutions of non-homogeneous conservation laws when the system admits stationary solutions are a consequence of the inability of the schemes to compensate the difference of the fluxes with the source terms to the input and output of each control volume. This is the case, for example, of Euler's equations with a geometric source term that represents the computation of the quasi-1D flow in ducts of variable cross section (see [13] or [14]), shallow water flows in an open channel, for whose integration many numerical techniques have been suggested in the literature (see [7], [8], [9] and [10], for example) or compressible axially symmetric flows in tubes with variable cross section (see [15] and [16]).

Numerical solutions for the Euler equations of the quasi-1D flow in ducts of variable cross-section have been important in Internal Combustion Engines (I.C.E.). The flow in the pipes of I.C.E. has some characteristics which make an accurate calculation very difficult. First, the unsteadiness of the reciprocating operation that leads to a periodical but strongly non steady flow. Secondly, compressibility plays an important role, therefore the flow must be treated as fully compressible, and also as multicomponent because of the great difference existing on the thermodynamic properties of the involved gases. And finally, the presence of shock waves and huge thermal discontinuities due to the difference of temperature between exhaust gases and fresh air. All this, combined with high flux velocities, makes the calculation of the flow in pipes of an I.C.E. a difficult problem to solve. Therefore, the research on numerical methods that could be used to efficiently solve this pseudo 1-D flow has been one of the main important topics in the area of engine modeling.

In this paper we use the technique introduced in [1] by the authors to extend some high-order schemes to quasi-1D flow in ducts of variable cross-section. This method allows include the source term in a divergence form, generating well-balanced schemes which preserve steady state solutions of hyperbolic conservation laws with source terms. To apply this technique a new flux, defined as the subtraction of the primitive function of the source term from the physical flux, is considered; so, the non-homogeneous problem is written as homogeneous. This strategy has also been used in [17] and [18] to the shallow water flows. In this work we describe the extension of the flux limiter technique and the HLL Riemann solver to the quasi-1D flow in ducts of variable cross-section. The firs method requires characteristic decomposition in order to extend the scalar problem to the vectorial case, while the HLL scheme does not need the characteristic decomposition.

The paper is organized as follows. Section 2 briefly recalls the governing equations of the flow in ducts of variable cross-section. Then, in Section 3, we detail the well-balanced flux limiter and the HLL Riemann schemes adapted to the quasi-1D flow. In Section 4 we will show numerical results of the flow in a convergent-divergent nozzle in order to enable the capacity of the schemes developed to capture stationary solutions associated with non-homogeneous conservation laws. Finally, in Section 5 we summarize the main conclusions of the paper.

2. Governing Equations

Equations for quasi-1D unsteady nozzle flows can be expressed in a conservative form as follows

$$\partial_t W + \partial_x F\left(W\right) = S(x, W) \tag{1}$$

where $W(x,t)$ represents the solution vector, $F(W)$ is the flux vector

$$W(x,t) = \begin{pmatrix} \rho A \\ \rho u A \\ \left(\rho \frac{u^2}{2} + \frac{p}{\gamma-1}\right) A \end{pmatrix} \quad , \qquad F(W) = \begin{pmatrix} \rho u A \\ \left(\rho u^2 + p\right) A \\ u \left(\rho \frac{u^2}{2} + p \frac{\gamma}{\gamma-1}\right) A \end{pmatrix} \tag{2}$$

and

$$S(x, W) = \begin{pmatrix} 0 \\ pA'(x) - g\rho A_l \\ q\rho A_l \end{pmatrix} \tag{3}$$

is the source vector including the effect of the cross section variation on the flow and the effect of wall friction and heat transfer on the energy and momentum equations.

This compact vector form includes the area in the solution vector and, as can be observed in Equation (3), the source terms in the continuity equation and in the energy equation are independent of the cross-section variation.

The above system, composed by the continuity, momentum and energy equations, is closed by the state equation

$$e = \rho \frac{u^2}{2} + \frac{p}{\gamma - 1}. \tag{4}$$

Here, the quantities ρ, u, p and e represent the density, velocity, pressure and total energy; A is the cross section, $A'\left(x\right)$ is the x derivative of A, γ denotes the specific heat ratio of the gas, q the term transferred to the walls, g the friction and A_l represents the wall surface per unit length, which coincides with the value of the duct diameter in this case ($A_l = A$). The flux Jacobian matrix is given by

$$J(W) = \frac{\partial F}{\partial W} = \begin{pmatrix} 0 & 1 & 0 \\ \frac{\gamma-3}{2} u^2 & (3-\gamma)u & \gamma - 1 \\ u\left(\frac{\gamma-1}{2}u^2 - H\right) & H - (\gamma-1)u^2 & \gamma u \end{pmatrix} \tag{5}$$

where H is the entalphy, which is given by

$$H = \frac{a^2}{\gamma - 1} + \frac{u^2}{2} \tag{6}$$

and a denotes the sound speed.

Hyperbolicity of the above system implies that the Jacobian matrix J is diagonalizable, with real eigenvalues. Therefore $D = LJR$, where D is the eigenvalues matrix, and the eigenvalues of J ($u - a$, u and $u + a$) will be on the diagonal of D. The matrix of right eigenvectors is defined by

$$R = \begin{pmatrix} 1 & 1 & 1 \\ u - a & u & u + a \\ H - ua & \frac{1}{2}u^2 & H + ua \end{pmatrix} \tag{7}$$

and the left eigenvectors matrix is given by

$$L = \left(\frac{\gamma - 1}{2a^3}\right) \begin{pmatrix} u\left(\frac{a^2}{\gamma-1} + \frac{1}{2}ua\right) & -\left(\frac{a^2}{\gamma-1} + ua\right) & a \\ a\left(\frac{2a^2}{\gamma-1} - u^2\right) & 2ua & -2a \\ ua\left(\frac{1}{2}u - \frac{a}{\gamma-1}\right) & \left(\frac{a^2}{\gamma-1} - ua\right) & a \end{pmatrix} \tag{8}$$

Finally, Jacobian matrix of the source vector to read as follows

$$\frac{\partial S}{\partial W} = \begin{pmatrix} 0 & 0 & 0 \\ \frac{\gamma-1}{2}\frac{A'}{A}u^2 - g & (1-\gamma)\frac{A'}{A}u & (\gamma - 1)\frac{A'}{A} \\ q & 0 & 0 \end{pmatrix} \tag{9}$$

The main cause of the conservation errors obtained with classical conservative schemes used for problems with cross-section constant when they are applied to pipes with variable cross-section is due to the use of density, momentum and energy as conserved variables, because if the cross-section is not constant along the pipe, the actual conserved variables are mass, mass flow rate and total energy. Furthermore, the flux terms $F(W)$ are the natural fluxes that correspond to mass and energy in 1-D flow, while the momentum equation establishes the equilibrium among the different forces that act on the control volume. Many errors are directly linked to the fact that some singular contribution has been omitted in the momentum equation. Indeed, the $pA'(x)$ term should always balance the second component of the flow vector [19], therefore it should be incorporated in a divergence form, since it really corresponds to the divergence of surface forces acting on the side walls of the control volume, and not a source term as it is usually treated. Here, the $pA'(x)$ term represents the reaction forces from the wall to the flow in pipes where the cross section varies and its evaluation also requires the integration of the product pdA over the control volume.

In particular, the source term associated with the variation of the cross-sectional area of the duct causes numerical errors in steady flow problems when an exact or approximate balance of the flux gradient and the source term is not achieved. The numerical techniques we propose are able to preserve steady states at the discrete level.

3. Description of Numerical Schemes

This Section is devoted to the formulation of numerical schemes based on the *homogeneous form* of the balance laws in order to ensure well-balancing properties. This technique, described in [1], and consisting in the transformation of the non-homogeneous problem into homogeneous through the introduction of a new flux formed by the physical flux and the primitive function of the source term, preserves directly the well-balancing properties needed to compute accurately steady state solutions for which the flux gradients are balanced by the source terms.

Two schemes have been adapted to compute the steady quasi-1D flows. On the one hand, the flux limiter technique, that is widely applied to homogeneous problems and which requires characteristic decomposition in order to extend the scalar problem to the vectorial case. This scheme has been adapted in [18] for shallow water flows following this methodology. On the other hand, we have extended the HLL Riemann solver [3] to the non-homogeneous problem in order to obtain a well-balanced scheme that does not need the characteristic decomposition.

3.1. Homogeneous form of the flux limiter technique

To design the flux limiter technique for the quasi-1D flow we first examine the scalar case and then construct the numerical flux function for the system case by implementing the scalar numerical flux in each characteristic field.

3.1.1. Scalar case

Let us consider the scalar non-homogeneous hyperbolic conservation law

$$\partial_t w + \partial_x f(w) = s(x) \tag{10}$$

that governs the evolution of the variable $w(x,t)$, being $f(w)$ the flux and $s(x)$ the source term, which we will first assume it depends only on x. Since we are interested in finding discretizations that recognize stationary solutions of (10), it can be observed that from the associated equation of a stationary state

$$\partial_x f(w) = s(x) \tag{11}$$

the $f(w)$ function could be written as

$$f(w) = K + \int_{x_0}^{x} s(z)dz \tag{12}$$

being K and x_0 constants. This expression indicates that to ensure the well-balance property, we need schemes with similar discretization for the flux that for the primitive function of the source term. With this aim, we denote

$$g(x,w) = f(w) - \int_{x_0}^{x} s(z)dz \tag{13}$$

that represents a new flux defined as difference of the primitive function of the source term and the physical flux. Now, Equation (10) takes the form

$$\partial_t w + \partial_x g(x,w) = 0 \tag{14}$$

independently of the chosen value for x_0.

With the above conversion from non-homogeneous to homogeneous problem we obtain two important objectives. On the one hand, the application of schemes already applied to the homogeneous case, widely studied, to the case of conservation laws with source term. However, the extension of some techniques may not be immediate due to the fact that now the new flux depends not only on w but also on the variable x. In order to design convenient methods for this problem we shall formulate the schemes with a similar structure that the homogeneous case. On the other hand, this transformation allows to treat the source term as a divergence term guaranteeing that the schemes recognize stationary solutions associated with the non-homogeneous problem.

Considering a uniform mesh, with cell sizes Δx and Δt, and by integrating Equation (10) over the rectangle $\left[x_{j-1/2}, x_{j+1/2}\right] \times [t_n, t_{n+1}]$, we obtain

$$\begin{aligned} w_j^{n+1} = w_j^n &- \frac{1}{\Delta x}\int_{t_n}^{t_{n+1}} \left(f\left(w\left(x_{j+1/2},t\right)\right) - f\left(w\left(x_{j-1/2},t\right)\right)\right)dt \\ &+ \frac{1}{\Delta x}\int_{t_n}^{t_{n+1}} \int_{x_{j-1/2}}^{x_{j+1/2}} s\left(x\right)dxdt \end{aligned} \tag{15}$$

where w_j represents an approximation of the average of the solution on the interval $\left[x_{j-1/2}, x_{j+1/2}\right]$ in the corresponding instant, that is

$$w_j^k = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} w(x,t_k)dx, \quad \text{for } k = n, n+1. \tag{16}$$

Taking into account the definition of g according to Equation (13), Equation (15) can be rewritten as

$$w_j^{n+1} = w_j^n - \frac{1}{\Delta x}\int_{t_n}^{t_{n+1}} \left(g\left(x_{j+1/2}, w\left(x_{j+1/2},t\right)\right) - g\left(x_{j-1/2}, w\left(x_{j-1/2},t\right)\right)\right)dt. \tag{17}$$

Therefore, limiting our scope only to the case of explicit techniques, we suggest schemes whose conservative expression is

$$w_j^{n+1} = w_j^n - \lambda\left[\overline{g}_{j+1/2}^n - \overline{g}_{j-1/2}^n\right] \tag{18}$$

where $\lambda = \dfrac{\Delta t}{\Delta x}$ and

$$\overline{g}^n_{j+1/2} = \overline{g}(x_{j-k+1}, \ldots, x_{j+k}, w^n_{j-k+1}, \ldots, w^n_{j+k}). \tag{19}$$

Let's notice that $\overline{g}$ denotes an average numerical flux constructed as the difference of the numerical flux associated with the function f and other numerical flux associated with the primitive function of the source term.

As a first application of this technique, we have the next formulation of the classic Lax-Wendroff scheme, presented in [1], for the numerical integration of Equation (10)

$$w^{n+1}_j = w^n_j - \lambda \left[g^{n+\frac{1}{2}}_{j+\frac{1}{2}} - g^{n+\frac{1}{2}}_{j-\frac{1}{2}} \right] \tag{20}$$

where the estimation of the new flux between two nodes in the middle instant is obtained, as in the homogeneous case, from a simple Taylor's development. That is to say,

$$g^{n+\frac{1}{2}}_{j+\frac{1}{2}} = \frac{1}{2} \left[g^n_j + g^n_{j+1} - \lambda \left.\frac{\partial f}{\partial w}\right|^n_{j+\frac{1}{2}} \left(g^n_{j+1} - g^n_j \right) \right] \tag{21}$$

being

$$g^n_i = f^n_i - \int_{x_{j-\frac{1}{2}}}^{x_i} s(z)dz \quad \text{for} \quad i = j,\ j+1 \tag{22}$$

and where we have chosen $x_0 = x_{j-\frac{1}{2}}$. Introducing now the notation

$$b_{i,k} = -\int_{x_i}^{x_k} s(z)dz \tag{23}$$

we can write Equation (21) as

$$g^{n+\frac{1}{2}}_{j+\frac{1}{2}} = \frac{1}{2} \left[f^n_j + b^n_{j-\frac{1}{2},j} + f^n_{j+1} + b^n_{j-\frac{1}{2},j+1} - \lambda \left.\frac{\partial f}{\partial w}\right|^n_{j+\frac{1}{2}} \left(f^n_{j+1} - f^n_j + b^n_{j,j+1} \right) \right] \tag{24}$$

The scheme defined by Equations (20)-(24) can be expressed through the next formulation

$$w^{n+1}_j = w^n_j - \lambda \left[\hat{g}_{j+\frac{1}{2}} - \hat{g}_{j-\frac{1}{2}} \right] - \lambda \left[b^n_{j-\frac{1}{2},j} + b^n_{j,j+\frac{1}{2}} \right] \tag{25}$$

where the flux in the middle $\hat{g}_{j+\frac{1}{2}}$ is calculated using only estimations of the source terms in the interval $[x_j, x_{j+1}]$

$$g^{LW}_{j+\frac{1}{2}} = \frac{1}{2} \left[f^n_j + f^n_{j+1} - b^n_{j,j+\frac{1}{2}} + b^n_{j+\frac{1}{2},j+1} - \alpha^n_{j+\frac{1}{2}} \left(f^n_{j+1} - f^n_j + b^n_{j,j+1} \right) \right]. \tag{26}$$

It is precisely this type of formulation, with a structure similar to that of the homogeneous case, that facilitates the extension of the schemes for the non-homogeneous case.

In the above expression, we have used the following notation

$$\alpha^n_{j+\frac{1}{2}} = \lambda \left.\frac{\partial f}{\partial w}\right|^n_{j+\frac{1}{2}} = \begin{cases} \lambda \frac{f^n_{j+1}-f^n_j}{w^n_{j+1}-w^n_j} & \text{if} \quad w^n_{j+1}-w^n_j \neq 0 \\ \lambda \left.\frac{\partial f}{\partial w}\right|^n_j & \text{if} \quad w^n_{j+1}-w^n_j = 0 \end{cases} \tag{27}$$

An identical development would allow us to deduce the formulation of the first-order upwind scheme on applying it to integrate Equation (10), defining $\hat{g}_{j+\frac{1}{2}}$ in (25) through the expression

$$g^{UP}_{j+\frac{1}{2}} = \frac{1}{2}\left[f^n_j + f^n_{j+1} - b^n_{j,j+\frac{1}{2}} + b^n_{j+\frac{1}{2},j+1} - \text{sign}\left(\alpha^n_{j+\frac{1}{2}}\right)\left(f^n_{j+1} - f^n_j + b^n_{j,j+1}\right)\right]. \tag{28}$$

Similarly, taking into account the construction of the flux limiters suggested by Sweby in [2] for the homogeneous case, we can extend this technique considering $\hat{g}_{j+\frac{1}{2}}$ in Equation (25) as

$$g^{SW}_{j+\frac{1}{2}} = g^{UP}_{j+\frac{1}{2}} + \chi(r_{j+\frac{1}{2}})\left(g^{LW}_{j+\frac{1}{2}} - g^{UP}_{j+\frac{1}{2}}\right) \tag{29}$$

where

$$r_{j+\frac{1}{2}} = \frac{\left(\text{sign}\left(\alpha_{j+\frac{1}{2}-\overline{s}}\right) - \alpha_{j+\frac{1}{2}-\overline{s}}\right)\Delta_{j+\frac{1}{2}-\overline{s}}\, g}{\left(\text{sign}\left(\alpha_{j+\frac{1}{2}}\right) - \alpha_{j+\frac{1}{2}}\right)\Delta_{j+\frac{1}{2}}\, g} \tag{30}$$

being $\overline{s} = \text{sign}(\alpha_{j+\frac{1}{2}})$ and

$$\Delta_{j+\frac{1}{2}-\overline{s}}\, g = f_{j+1-\overline{s}} - f_{j-\overline{s}} + b_{j-\overline{s},j+1-\overline{s}} \tag{31}$$

With respect to $\chi(r)$ it can be any of the limiters found in the literature (see [2] and [5]). Particularly, we have chosen for the calculations of the present paper the superbee limiter:

$$\chi_{SB}(r) = \max\{0, \min\{2r, 1\}, \min\{r, 2\}\} \tag{32}$$

In summary, we can write the extension of the schemes proposed as

$$w^{n+1}_j = w^n_j - \lambda\left[\hat{g}_{j+\frac{1}{2}} - \hat{g}_{j-\frac{1}{2}}\right] - \lambda\left[b^n_{j-\frac{1}{2},j} + b^n_{j,j+\frac{1}{2}}\right] \tag{33}$$

with

$$\hat{g}_{j+\frac{1}{2}} = \frac{1}{2}\left[f^n_j + f^n_{j+1} - b^n_{j,j+\frac{1}{2}} + b^n_{j+\frac{1}{2},j+1} - \Phi\left(\alpha^n_{j+\frac{1}{2}}\right)\left(f^n_{j+1} - f^n_j + b^n_{j,j+1}\right)\right], \tag{34}$$

being

$\hat{g}_{j+\frac{1}{2}} = g^{LW}_{j+\frac{1}{2}}$ when $\Phi(x) = x$ (Lax-Wendroff scheme)

$\hat{g}_{j+\frac{1}{2}} = g^{UP}_{j+\frac{1}{2}}$ when $\Phi(x) = \text{sign}(x)$ (first-order upwind method)

$\hat{g}_{j+\frac{1}{2}} = g^{SW}_{j+\frac{1}{2}}$ when $\Phi(x) = \text{sign}(x) + \chi(r)\left[x - \text{sign}(x)\right]$ (flux limiter)

Introducing the notation

$$
\begin{aligned}
g_j^- &= f_j^n + b_{j-\frac{1}{2},j}^n \\
g_j^+ &= f_j^n - b_{j,j+\frac{1}{2}}^n
\end{aligned} \tag{35}
$$

we have

$$
g_{j+1}^- - g_j^+ = f_{j+1}^n - f_j^n + b_{j,j+1}^n \tag{36}
$$

and $\hat{g}_{j+\frac{1}{2}}$ in Equation (34) can be written by

$$
\hat{g}_{j+\frac{1}{2}} = \frac{1}{2}\left\{g_j^+ + g_{j+1}^- - \Phi\left(\alpha_{j+\frac{1}{2}}\right)\left(g_{j+1}^- - g_j^+\right)\right\} \tag{37}
$$

Notice that with this formulation of the schemes, Equations (33) – (37) provide easily computable numerical flux functions which have a similar structure that the homogeneous case and where the source terms are straightforward discretized to achieve perfect balance with flux terms at steady states.

In order to define a fully second order scheme when the source term s in Equation (10) depends on x and $w(x,t)$, we must take into account two additional considerations which have been pointed out in [18], where an extension to shallow water equations has been presented. On the one hand, a new term has to be included in Equation (33) which read as follows

$$
w_j^{n+1} = w_j^n - \lambda\left[\hat{g}_{j+\frac{1}{2}} - \hat{g}_{j-\frac{1}{2}}\right] - \lambda\left[b_{j-\frac{1}{2},j}^n + b_{j,j+\frac{1}{2}}^n\right] - \lambda\left[h_{j+\frac{1}{2}}^n + h_{j-\frac{1}{2}}^n\right] \tag{38}
$$

This term arises from the discretization of the source term with respect to the time (see [20])

$$
h_{j+\frac{1}{2}}^n = \frac{\Delta t}{4}\left.\frac{\partial s}{\partial w}\right|_{j+\frac{1}{2}}^n \left(f_{j+1}^n - f_j^n + b_{j,j+1}^n\right) \tag{39}
$$

On the other hand, we must use a quadrature rule with at least second order accuracy to approximate

$$
b_{i,k}^n = -\int_{x_i}^{x_k} s(z, w^n)dz \tag{40}
$$

As it has been shown in [20], we observe that the use of a trapezoidal rule or other quadrature rule, at least second order accurate, to approximate $b_{i,k}^n$ together with all the differences in the scheme are expressed as flux differences balancing with the source terms, i.e., with terms of the form $\left(f_{j+1}^n - f_j^n + b_{j,j+1}^n\right)$ will be sufficient to ensure the C-property [7].

It is important to point out that there are not significant differences in numerical results when other quadrature rules have been used to approximate $b_{i,k}^n$. However, the inclusion of the source term as a divergence term is particularly important in order to ensure the balance of the flux and source terms at steady since allows us to design well-balanced schemes in a rather straightforward way.

In fact, the above suggested schemes preserve stationary solutions associated with the conservation law (10). Let's observe that substituting in each case the definition of $\hat{g}$ in the expression (33), we obtain

$$\begin{aligned} w_j^{n+1} &= w_j^n - \frac{\lambda}{2}\left[1-\Phi\left(\alpha_{j+\frac{1}{2}}^n\right)+\frac{\Delta t}{2}\left.\frac{\partial s}{\partial w}\right|_{j+\frac{1}{2}}^n\right]\left(f_{j+1}^n-f_j^n+b_{j,j+1}^n\right) \\ &\quad - \frac{\lambda}{2}\left[1+\Phi\left(\alpha_{j-\frac{1}{2}}^n\right)+\frac{\Delta t}{2}\left.\frac{\partial s}{\partial w}\right|_{j-\frac{1}{2}}^n\right]\left(f_j^n-f_{j-1}^n+b_{j-1,j}^n\right) \end{aligned} \tag{41}$$

Therefore, if w_j^n is a second order approximation to the steady-state solution of (10), that is to say, it is satisfied

$$f_{j+1}^n-f_j^n+b_{j,j+1}^n = O\left(\Delta x^3\right) \quad , \forall j \tag{42}$$

where $b_{j,j+1}^n$ represents a quadrature rule that is at least second order accurate to approximate the integral of Equation (40), then

$$w_j^{n+1} = w_j^n + O\left(\Delta x^3\right) \tag{43}$$

and w_j^{n+1} approximates the stationary solution with the same accuracy, at least.

3.1.2. Vectorial case

This Section will extend previous schemes to solve non-homogeneous hyperbolic conservation law systems expressed as

$$\partial_t W + \partial_x F\left(W\right) = S(x,W) \tag{44}$$

where $W = W(x,t)$ represents the flow variables, $F(W)$ the fluxes vector and $S(x,W)$ denotes the source term. All vectors have m components.

Extension of the scalar case to systems of conservation laws is based on field-by-field decompositions. We first consider linear, constant coefficient case and the source term depending only on x,

$$\partial_t W + J\partial_x W = S(x) \tag{45}$$

being the Jacobian matrix J constant.

We notice that Equation (45) can be written as

$$\partial_t W + \partial_x G\left(x,W\right) = 0 \tag{46}$$

with $G(x,W)$ defined by

$$G(x,W) = F(W) - \int_{x_{j-\frac{1}{2}}}^{x} S(z)dz. \tag{47}$$

which can be considered as a new flux formed by subtracting from the physical flow the primitive of the source term.

Since the system (45) is hyperbolic, the Jacobian matrix J is diagonalizable with real eigenvalues. Therefore, if R is the matrix formed by the columns of the right eigenvectors, the diagonalized form of J is given by

$$D = LJR, \quad \text{with } L = R^{-1} \tag{48}$$

being

$$D = \operatorname{diag}(\lambda_k), \;\; k = 1 \dots m \tag{49}$$

the diagonal matrix of eigenvalues of J.

We can solve the system (45) by transforming it into the characteristic variables

$$U = LW \tag{50}$$

Therefore, multiplying Equation (45) by L, we obtain

$$\partial_t U + D \partial_x U = LS. \tag{51}$$

Since D is diagonal, this is a decoupled set of non-homogeneous scalar equations. Now, Equation (51) can be solved by applying to each scalar characteristic equation the scheme presented in the previous Section. Then, the scheme expressed in terms of the original variables can be recovered by multiplying the resulting discretized system of equations by R. Furthermore, for the case where J is not constant, using an average (Roe average, by example) for $R_{j+\frac{1}{2}}$, $D_{j+\frac{1}{2}}$ and $L_{j+\frac{1}{2}}$, we can write

$$W_j^{n+1} = W_j^n - \lambda \left[\hat{G}_{j+\frac{1}{2}} - \hat{G}_{j-\frac{1}{2}} \right] - \lambda \left[B^n_{j-\frac{1}{2},j} + B^n_{j,j+\frac{1}{2}} \right] \tag{52}$$

where

$$\begin{aligned} \hat{G}_{j+\frac{1}{2}} = \frac{1}{2} \Big\{ & F_j^n + F_{j+1}^n - B^n_{j,j+\frac{1}{2}} + B^n_{j+\frac{1}{2},j+1} - \\ & - R_{j+\frac{1}{2}} \Phi(D^\chi_{j+\frac{1}{2}}) L_{j+\frac{1}{2}} \left[F^n_{j+1} - F^n_j + B^n_{j,j+1} \right] \Big\} \end{aligned} \tag{53}$$

or, equivalently,

$$\hat{G}_{j+\frac{1}{2}} = \frac{1}{2} \left\{ G_j^+ + G_{j+1}^- - R_{j+\frac{1}{2}} \Phi(D^\chi_{j+\frac{1}{2}}) L_{j+\frac{1}{2}} \left[G^-_{j+1} - G^+_j \right] \right\} \tag{54}$$

denoting

$$G_j^- = F_j^n + B^n_{j-\frac{1}{2},j} \tag{55}$$

$$G_j^+ = F_j^n - B^n_{j,j+\frac{1}{2}} \tag{56}$$

and $\Phi(D^\chi_{j+\frac{1}{2}})$ a diagonal matrix, whose diagonal elements are defined by

$$\operatorname{sign}\left(\alpha^k_{j+\frac{1}{2}}\right) + \chi\left(r^k_{j+\frac{1}{2}}\right) \left[\left(\alpha^k_{j+\frac{1}{2}}\right) - \operatorname{sign}\left(\alpha^k_{j+\frac{1}{2}}\right) \right] \tag{57}$$

being

$$r^k_{j+\frac{1}{2}} = \frac{\left(\text{sign}\left(\alpha^k_{j+\frac{1}{2}-\overline{s}^k}\right) - \left(\alpha^k_{j+\frac{1}{2}-\overline{s}^k}\right)\right)\delta g^k_{j+\frac{1}{2}-\overline{s}^k}}{\left(\text{sign}\left(\alpha^k_{j+\frac{1}{2}}\right) - \left(\alpha^k_{j+\frac{1}{2}}\right)\right)\delta g^k_{j+\frac{1}{2}}} \tag{58}$$

where $\overline{s}^k = \text{sign}\left(\alpha^k_{j+\frac{1}{2}}\right)$ and $\alpha^k = \frac{\Delta t}{\Delta x}\lambda_k$. We notice that $\delta g^k_{j+\frac{1}{2}}$ can be viewed as the components of the vector $F_{j+1} - F_j + B_{j,j+1}$ in the coordinate system $\left\{R^k_{j+\frac{1}{2}}\right\}$, i.e. it denotes the $k-$th component of the vector

$$L_{j+\frac{1}{2}}(F_{j+1} - F_j + B_{j,j+1}). \tag{59}$$

As before, the above scheme can be extended to the case in which the source term depends on x and $W(x,t)$, by replacing Equation (52) with

$$W^{n+1}_j = W^n_j - \lambda\left[\hat{G}_{j+\frac{1}{2}} - \hat{G}_{j-\frac{1}{2}}\right] - \lambda\left[B^n_{j-\frac{1}{2},j} + B^n_{j,j+\frac{1}{2}}\right] - \lambda\left[H^n_{j-\frac{1}{2}} + H^n_{j+\frac{1}{2}}\right] \tag{60}$$

where

$$H^n_{j+\frac{1}{2}} = \frac{\Delta t}{4}\left.\frac{\partial S}{\partial W}\right|^n_{j+\frac{1}{2}}\left(F^n_{j+1} - F^n_j + B^n_{j,j+1}\right) \tag{61}$$

and taking a trapezoidal rule or any quadrature rule at least second order accurate for each component of

$$B^n_{i,k} = -\int_{x_i}^{x_k} S(z, W^n)dz. \tag{62}$$

Remark 1. *The scheme* $(60)-(53)$ *where the matrix* $\Phi(D^\chi_{j+\frac{1}{2}})$ *is chosen to be*

$$\text{diag}\left(\text{sign}\left(\alpha^k_{j+\frac{1}{2}}\right)\right) \tag{63}$$

can be seen as the extension of the first-order upwind scheme for non-homogeneous conservation laws. Moreover, the choice

$$\Phi(D^\chi_{j+\frac{1}{2}}) = \text{diag}\left(\alpha^k_{j+\frac{1}{2}}\right) \tag{64}$$

gives the natural extension of the Lax-Wendroff scheme for this case.

The *homogeneous form* transformation applied in this paper allowed the authors extend the second-order TVD schemes defined in [4] to the non-homogeneous case with stationary solutions through a formulation of the same type (see [1]).

Finally, to implement the scheme defined by Equations $(53)-(60)$ to approximate the solution of the system (1) which describes the quasi-1D unsteady compressible flow in ducts with varying cross-section, we need some intermediate values for u, H and p. For this, we apply the Roe's linearization technique described in [21]. For our case, this averaging can be written as

$$
\begin{aligned}
\chi_{j+\frac{1}{2}} &= \sqrt{\tfrac{\rho_{j+1}A_{j+1}}{\rho_j A_j}} \quad &,& \quad u_{j+\frac{1}{2}} = \frac{\chi_{j+\frac{1}{2}} u_{j+1} + u_j}{\chi_{j+\frac{1}{2}} + 1} \\
H_{j+\frac{1}{2}} &= \frac{\chi_{j+\frac{1}{2}} H_{j+1} + H_j}{\chi_{j+\frac{1}{2}} + 1} \quad &,& \quad \rho_{j+\frac{1}{2}} = \sqrt{\rho_j \rho_{j+1}} \\
\rho_{j+\frac{1}{2}} A_{j+\frac{1}{2}} &= \sqrt{\rho_j A_j \rho_{j+1} A_{j+1}} \quad &,& \quad p_{j+\frac{1}{2}} = \tfrac{1}{\gamma}\left(\rho_{j+\frac{1}{2}} a^2_{j+\frac{1}{2}}\right)
\end{aligned}
\tag{65}
$$

Following the averages determined above for $u_{j+\frac{1}{2}}$ and $H_{j+\frac{1}{2}}$, a natural approximation of the Jacobian matrices in the middle, $\frac{\partial F}{\partial W}\big|_{j+\frac{1}{2}}$ and $\frac{\partial S}{\partial W}\big|_{j+\frac{1}{2}}$, as well as left and right eigenvectors matrices, $L_{j+\frac{1}{2}}$ and $R_{j+\frac{1}{2}}$, respectively, can be obtained from expressions (5) − (9).

Finally, to estimate the source terms B over the control volume $[k, i]$, we need the above averages of p and ρA and then we propose a simple arithmetic average for the third component and the following discretization for the second:

$$
b^{(2)}_{k,i} = p_{\frac{k+i}{2}}(A_k - A_i) + (\Delta x)(g\rho A)_{\frac{k+i}{2}} \ . \tag{66}
$$

We note that, in contrast with [1], the upwinding of the discretization of the schemes described in this Section is based on the characteristic speeds derived from the homogeneous flux.

3.2. Homogeneous form of the HLL Approximate Riemann solver

In this Section the HLL approximate Riemann solver, proposed by Harten, Lax and van Leer in [3], has been adapted to calculate the quasi-1D nozzle flows. The HLL scheme assumes only one constant intermediate state between the left wave and the right wave and does not need characteristic decomposition of the flux difference. For the non-homogeneous problems, the classical HLL numerical scheme converges towards a numerical steady state which does not correspond to the physical one.

The key step in the extension of the HLL scheme to Equation (1) in order to obtain a conservative and well-balanced scheme is the formulation described in previous sections, which allows to write the scheme with an expression similar to the homogeneous case, like as

$$
W^{n+1}_j = W^n_j - \lambda\left[\hat{G}_{j+\frac{1}{2}} - \hat{G}_{j-\frac{1}{2}}\right] - \lambda\left[B^n_{j-\frac{1}{2},j} + B^n_{j,j+\frac{1}{2}}\right] - \lambda\left[H^n_{j-\frac{1}{2}} + H^n_{j+\frac{1}{2}}\right] \tag{67}
$$

with the intercell flux defined as

$$
\hat{G}_{j+\frac{1}{2}} = \begin{cases} G^+_j & \text{if} \quad \lambda_m(j) \geq 0 \\ G^-_{j+1} & \text{if} \quad \lambda_M(j) \leq 0 \\ G^* & , \quad \text{otherwise} \end{cases} \tag{68}
$$

where $\lambda_m(j)$ and $\lambda_M(j)$ are left and right wave speeds, respectively,

$$\begin{aligned}\lambda_m(j) &= \min\left\{u_j - a_j \ , \ u_{j+\frac{1}{2}} - a_{j+\frac{1}{2}}\right\} \\ \lambda_M(j) &= \max\left\{u_{j+1} + a_{j+1} \ , \ u_{j+\frac{1}{2}} + a_{j+\frac{1}{2}}\right\}\end{aligned} \tag{69}$$

Therefore, the solution of the HLL solver consists of three constant states separated by two characteristics $\lambda_m(j)$ and $\lambda_M(j)$. Furthermore,

$$\begin{aligned}G^-_{j+1} &= F^n_{j+1} + B^n_{j+\frac{1}{2},j+1} \\ G^+_j &= F^n_j - B^n_{j,j+\frac{1}{2}}\end{aligned} \tag{70}$$

include the effect of the source term, in contrast with the classical HLL scheme.

The numerical flux in the intermediate region G^* can be obtained by considering the two following Rankine-Hugoniot conditions

$$\begin{aligned}G^* - G^+_j &= \lambda_m(j)\left(W^* - \bar{W}_j\right) \\ G^-_{j+1} - G^* &= \lambda_M(j)\left(\bar{W}_{j+1} - W^*\right)\end{aligned} \tag{71}$$

By eliminating the W^* term in the above equations, it gives

$$G^* = \frac{\lambda_M(j)G^+_j - \lambda_m(j)G^-_{j+1}}{\lambda_M(j) - \lambda_m(j)} + \frac{\lambda_M(j)\lambda_m(j)}{\lambda_M(j) - \lambda_m(j)}\left(\bar{W}_{j+1} - \bar{W}_j\right) \tag{72}$$

Here, the modified difference of the flow variables must satisfy the following relation

$$\bar{W}_{j+1} - \bar{W}_j = W^n_{j+1} - W^n_j + J^{-1}_{j+\frac{1}{2}} B^n_{j,j+1} \tag{73}$$

in order to preserve the balance of the flux and source terms at steady states.

For the quasi-1D unsteady flow through a duct with variable cross-section the modified difference $\bar{W}_{j+1} - \bar{W}_j$ can be expressed by

$$\bar{W}_{j+1} - \bar{W}_j = W_{j+1} - W_j + \begin{bmatrix} \gamma \dfrac{b^{(2)}_{j,j+1}}{\lambda_m(j)\lambda_M(j)} \\ 0 \\ \dfrac{b^{(2)}_{j,j+1}}{1-\gamma}\left(1 + \dfrac{\gamma(3-\gamma)}{2} \cdot \dfrac{u^2_{j+\frac{1}{2}}}{\lambda_m(j)\lambda_M(j)}\right) \end{bmatrix} \tag{74}$$

The assumption of constant values for G^+_j, G^-_{j+1}, $\bar{W}_j$ and $\bar{W}_{j+1}$ in Equation (68) results in spatially first-order accuracy. In order to obtain a non-oscillatory second-order spatial accuracy method we can instead allow these values for each component to vary linearly in space, such that

$$\begin{aligned}\hat{q}_j &= q_j + \tfrac{1}{2}\min\bmod\left\{q_{j+1} - q_j, q_j - q_{j-1}\right\} \\ \hat{q}_{j+1} &= q_{j+1} - \tfrac{1}{2}\min\bmod\left\{q_{j+1} - q_j, q_{j+2} - q_{j+1}\right\}\end{aligned} \tag{75}$$

being $\hat{q}$ any approximation for $\bar{w}, g^{\pm}$, components of $\bar{W}$ and $G^{\pm}$, respectively. The minmod function is defined as the argument with smaller value if all arguments have the same sign and otherwise it is zero.

We would like to emphasize that one of the main advantages of the proposed scheme is its simplicity because of the system of the balance laws can be solved component-wise.

4. Numerical Results

In order to demonstrate the performance of the previously described methods some computations are shown using the next three tests. The purpose of the first test is to illustrate the well-balanced property of the schemes in order to preserve a steady solution.

Second and third tests involve unsteady flows and have been proposed with the aim of evaluating the ability of numerical schemes to converge with the time towards the steady state. The interest of the third problem is to study the accuracy of the numerical methods.

4.1. Preservation of steady states

To give a numerical validation of the well-balanced property, we consider the test proposed in [22], where the following initial data are chosen in order to guarantee a steady solution:

$$\begin{array}{c} A_L = 1.0,\ \rho_L = 1.0,\ p_L = 1.0,\ u_L = 1.0 \\ A_R = 1.1,\ \rho_R = 1.1314126,\ p_R = 1.1886922,\ u_R = 0.8035007 \end{array} \tag{76}$$

The initial discontinuity of the Riemann problem is located at $x = 0.4$. As is described in [22], the right state given above has been obtained by prescribing $A_R = 1.1$, and then enforcing Riemann invariants (mass flow rate, enthalpy and entropy) of the steady state to be constants.

For this case, the initial condition is a steady state that should be preserved. We check whether the numerical values for the mass flow rate ($\rho u A$) computed with the adapted flux limiter scheme, described by Eqs. (60)-(53), and with the HLL method, given by Eqs. (67)-(68), are round-off errors. For this, we run the steady state problem with several machine precisions (single, double and quadruple) and show, in Table 1, the L^1-errors for the mass flow rate with respect to the exact solution for the steady state ($\rho u A = 1$). Numerical results have been obtained with 1000 nodes and about 1000 time iterations.

As can be seen in Table 1, the errors are always of the order of the chosen machine accuracy, checking that the well-balanced schemes perfectly preserve the initial data.

4.2. Convergent-divergent nozzle

This test, proposed by the authors in [1], involves the convergent-divergent nozzle shown in Fig. 1.

Precision	Adapted Flux limiter	HLL extension
Single	$4.25E-07$	$8.22E-07$
Double	$3.22E-16$	$1.15E-15$
Quadruple	$2.03E-34$	$7.23E-34$

Table 1: L^1-errors with different precisions for the stationary mass flow rate solution ($\rho u A$) for the problem described in Section 4.1.

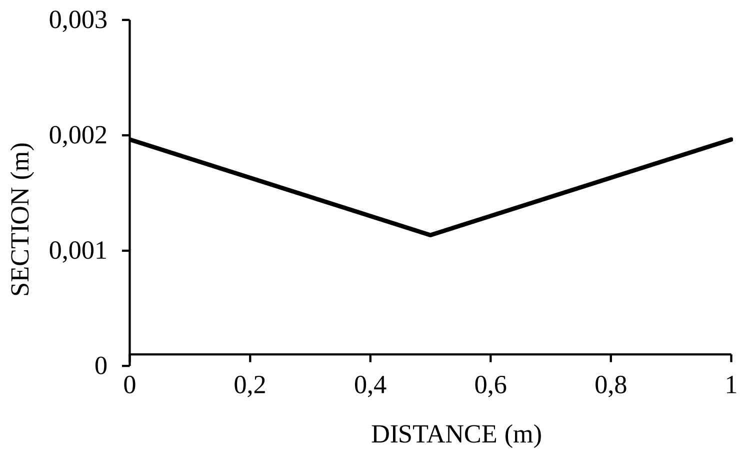

Figure 1: Convergent-divergent nozzle dimensions.

This is a nozzle connecting two atmospheres to different states. Initially, the duct is in the same conditions as the left atmosphere and is separated from the right atmosphere by a membrane. The transient begins when the membrane breaks, evolving over time to reach the stationary solution. The schemes have been tested numerically through the steady solution finally reached compared with the exact solution. Inside the pipe and at both ends, homentropic flow has always been assumed to make possible the computation of the exact solution. The nozzle, illustrated in Fig. 1, has length of 1 m, a diameter of 0.05 m at both sides and throat diameter of 0.038 m. The conditions of the calculation have been 2 bars of pressure and 300 K of temperature on the left atmosphere, whereas the right atmosphere has a pressure of 1.5 bar, so that a shock occurs inside the duct. Numerical results have been obtained with 51 nodes.

For this problem, the cross-section variation, included as a source term, has a significant influence on the flow. The transition from subsonic to supersonic velocity takes place at the throat and a sonic shock occurs in the divergent part of the nozzle. For this reason, it is essential to use a well-balanced and non oscillatory technique but at least of the second-order accuracy. Unbalancing schemes can destroy the convergence towards the steady state.

In Figures 2 and 3, the calculated pressure and velocity of the steady state so-

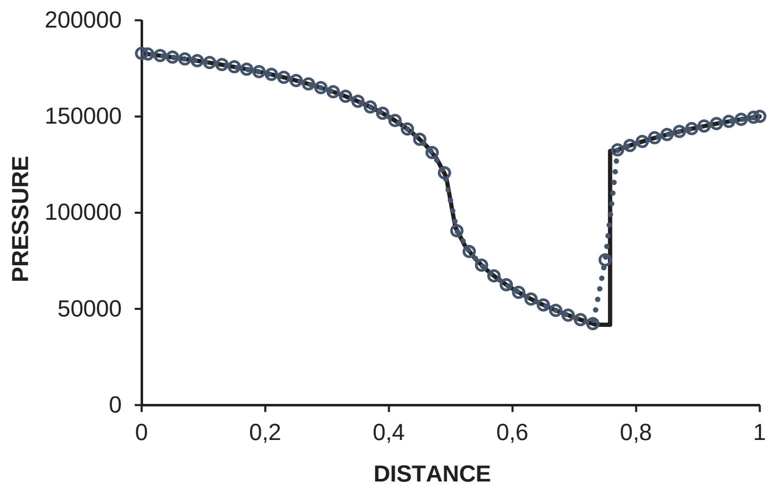

Figure 2: Steady pressure results of the nozzle of Fig. 1 obtained with the flux limiter extension, given by Eqs. (60)-(53), using 51 nodes.

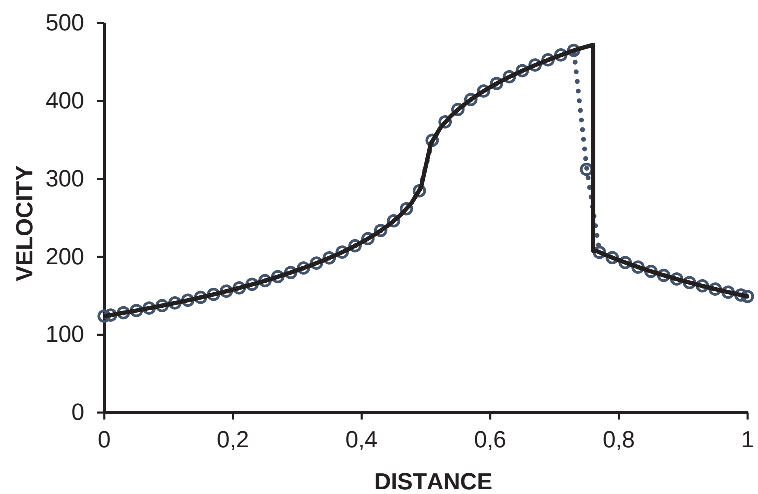

Figure 3: Steady velocity results of the nozzle of Fig. 1 obtained with the flux limiter extension, given by Eqs. (60)-(53), using 51 nodes.

lution for the convergent-divergent nozzle with the adapted flux limiter scheme, described by Eqs. (60)-(53), are shown. Numerical results are compared with the exact solution, depicted by the solid line. As can be observed in these figures, the pressure and velocity obtained with the second-order flux limiter method adjust quite well to the exact solution in most of the pipe, leading numerical results very close to the exact solutions, capturing, both the position and the strength of the shock very well. Only the shock point is wrong but no entropy violating solutions are obtained. The numerical wrong shock point appears because, on the control volume where the shock is located, the calculation of the flow properties in the middle is based on an average value between subsonic and supersonic states.

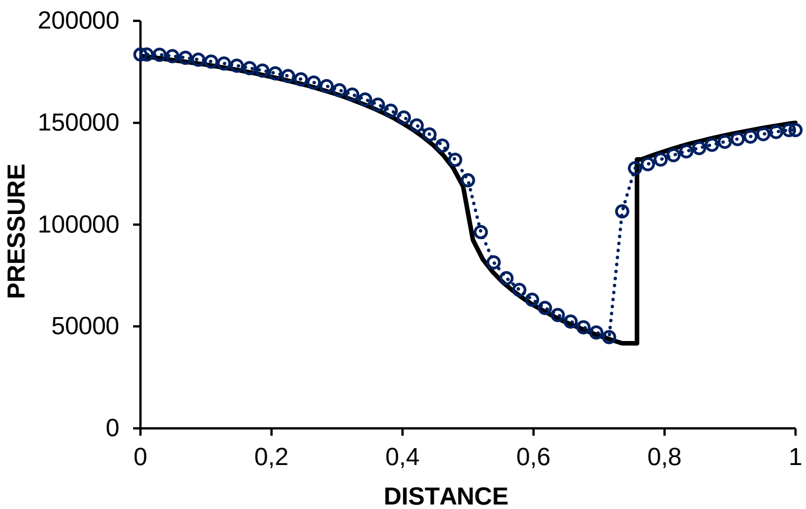

Figure 4: Steady pressure results of the nozzle of Fig. 1 obtained with the extension of the first-order HLL scheme, given by Eqs. (67)-(68), using 51 nodes.

Fig. 4 shows the pressure steady solution obtained for the above described convergent-divergent nozzle problem with the adapted HLL approximate Riemann solver described by Eqs. (67)-(68). However, in this case, numerical results are less accurate throughout the entire pipe because the scheme is only first-order accurate, therefore an extension to second order is necessary. Figs. 5 and 6 show both the pressure and velocity steady solution with the second-order spatial extension obtained using for each component to vary linearly in space with a minmod limiter (Equation (75)) to prevent the formation of the spurious oscillations.

As can be seen, the second-order extension of the HLL scheme gives much better results that the firs-order version, leading to a good approximation of the exact solution along the pipe except in the shock point where shows a wrong numerical solution. Just like the adapted flux limiter scheme, this is

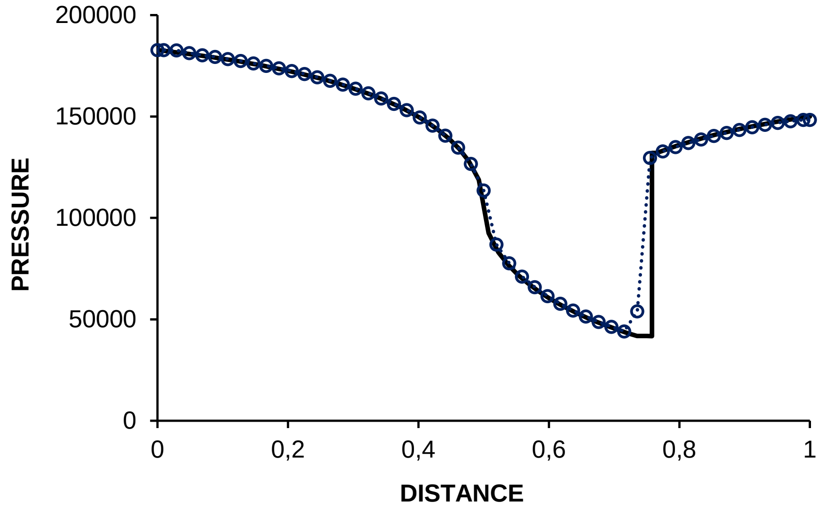

Figure 5: Steady pressure results of the nozzle of Fig. 1 obtained with the second-order extension of the HLL scheme, given by Eqs. (67)-(68), using 51 nodes.

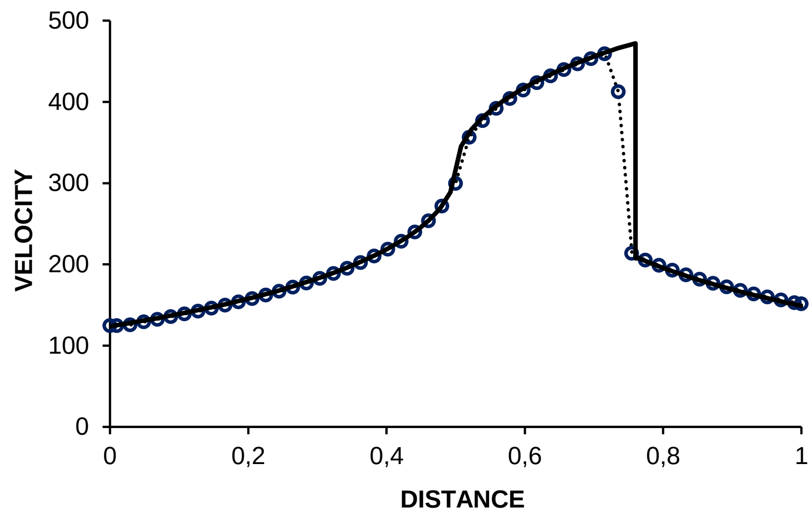

Figure 6: Steady velocity results of the nozzle of Fig. 1 obtained with the second-order extension of the HLL scheme, given by Eqs. (67)-(68), using 51 nodes.

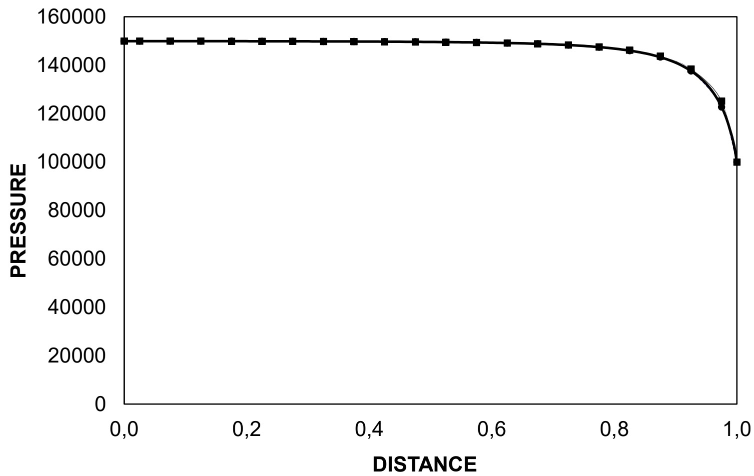

Figure 7: Steady pressure results for the nozzle of Section 4.3.

consequence of the use of averaged values in computing the numerical solution at cell interfaces between subsonic and supersonic fluid states and therefore it leads to a solution that is not physically real at the shock point.

4.3. Convergent conical nozzle

Finally, in order to check the accuracy of the schemes for smooth solutions, we consider a test that involves a convergent conical nozzle, with the following geometrical dimensions: 1 m length, 0.05 m diameter at the left side and 0.01 m at the right side.

The analyzed flow case is again the steady flow corresponding to a release of pure air through the nozzle, from the left atmosphere at 1.5 bar of pressure and 300 K of temperature to the right atmosphere at 1 bar of pressure. The analyzed solution is the pressure at the steady state achieved at $t = 0.06$ s.

Pressure obtained with the adapted flux limiter (squares), described by Eqs. (60)-(53), using 22 nodes, and with the HLL method (circles), given by Eqs. (67)-(68), are shown in Figure 7, in comparison with the exact solution (solid line). As can be seen, both methods yield similar results and show very good agreement with the exact solution.

Table 2 contains the L^1-errors and numerical orders of accuracy for the pressure solution of the convergent conical nozzle problem. We can see that the second order accuracy is achieved. Although numerical results obtained with the flux limiter extension show a better prediction, the difference is not great.

Number nodes	Error	Order	Error	Order
	Adapted Flux limiter		HLL extension	
40	$3.12E-03$		$1.93E-03$	
80	$7.25E-04$	2.10	$5.16E-04$	1.90
160	$2.03E-04$	1.83	$1.53E-04$	1.75
320	$5.03E-05$	2.01	$4.33E-05$	1.82

Table 2: L^1-errors of pressure and numerical orders of accuracy for the solution of the convergent nozzle test.

5. Conclusions

In the present study we have dealt with the simulation of quasi-1D unsteady compressible flow in a nozzle with variable cross-section. For this, we base on a technique described by the authors in [1] which consists in the transformation of the conservation laws system with source terms in homogeneous system. To do this, a new flux function has been introduced, which is defined by subtracting the primitive function of the source term from the physical flux. This change automatically preserves the balance among the source terms and the fluxes, required to assure the convergence to stationary solutions associated with non-homogeneous systems and indicates a natural way to apply to this type of problems schemes well-known for the homogeneous case. However, the extension of such techniques is not immediate in most cases and a new formulation for these schemes is necessary.

Particularly, we have extended the flux limiter technique and the HLL approximate Riemann solver to simulate quasi-1D nozzle flows. The constructed schemes are well-balanced in the sense that they preserve all stationary states [7]. Numerical results applied to a convergent-divergent nozzle, and valid for all quasi-1D geometries, indicate that the proposed schemes are very robust and capable of accurately capturing stationary solutions. Also, the advantage of the quasi-1D approach leads to CPU compute times that are really low compared to a multidimensional technique. Although numerical results are slightly more accurate with the adapted flux limiter technique, the extension to systems in this case is carried out by componentwise application of the scalar framework. However, the HLL scheme method does not need the field-by-field characteristic decomposition. Thus, a considerable amount of simplicity and robustness is gained while retaining the second-order resolution and gives to a well-balanced scheme.

It should be added that the numerical schemes detailed in this work could in fact be applicable to other type of non-homogeneous systems of PDEs in which the source term plays an important role in the solution, where the balance between flux and source term is necessary to reach steady state solutions.

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