AN ALTERNATIVE NUMERICAL PROCEDURE FOR SIMULATING MULTICOMPONENT FLOWS IN THE ATMOSPHERE

Eliane Maracajá Porto, eliane@lncc.br
Laboratory of Theoretical and Applied Mechanics (LMTA), Mechanical Engineering Graduate Program
Universidade Federal Fluminense, Rua Passo da Pátria 156, 24210-240, Niterói, RJ, Brazil
Laboratório Nacional de Computação Científica, Petrópolis/RJ, Brazil

Maria Laura Martins-Costa*, laura@mec.uff.br
Laboratory of Theoretical and Applied Mechanics (LMTA), Mechanical Engineering Department
Universidade Federal Fluminense, Rua Passo da Pátria 156, 24210-240, Niterói, RJ, Brazil

Rogério M. Saldanha da Gama, rsgama@terra.com.br
Mechanical Engineering Department, Universidade do Estado do Rio de Janeiro
Rua São Francisco Xavier, 524, 20550-013, Rio de Janeiro, RJ, Brazil

Abstract. *This article presents an alternative procedure to treat nonlinear hyperbolic systems. A preliminary hyperbolic model describes transport phenomena in an atmosphere, accounting for the propagation of gases, by including a source term representing production or destruction of gases due to chemical reactions. The resulting mathematical description consists of a nonlinear hyperbolic system of n+2 partial differential equations representing mass and momentum conservation for the multicomponent mixture of gases and air and n mass balance equations for the gases. This system simulation is performed by combining Glimm's scheme and an operator splitting technique to deal with the non-homogeneous part of the hyperbolic operator. An approximate Riemann solver is used, instead of the standard procedure to implement Glimm's method for advancing in time, which suffers from the disadvantage of requiring a complete solution of the associated Riemann problem. The alternative procedure employed in this article consists in approximating the solution of the associated Riemann problem by piecewise constant functions always satisfying the jump condition – thus circumventing the requirement of an analytical solution for the Riemann problem and giving rise to an approximation easier to implement with lower computational cost. Comparison with the standard procedure, employing the complete solution of the associated Riemann problem for implementing Glimm's scheme, has shown good agreement.*

Keywords*: Riemann solver, shock waves, multicomponent transport, piecewise constant approximation, operator splitting.*

1. INTRODUCTION

Although most transport phenomena description involves parabolic or elliptic partial differential equations which always admit regular solutions – whose simulation may employ well known numerical tools like finite elements, finite differences or finite volumes – there are several problems in Mechanics, like inviscid compressible flows or flows through unsaturated porous media that are mathematically represented by hyperbolic systems. These systems allow very realistic descriptions, since the propagation of any quantity – or information – in real natural phenomena is characterized by a finite speed; however they may not admit a regular solution, but a generalized solution involving shock waves, requiring specific numerical tools, such as, for instance, Glimm's scheme or Godunov's one, in order to account for their discontinuous nature.

Glimm's scheme is a reliable method with mathematically ensured accuracy (Glimm, 1965; Chorin, 1976), based on a theory presenting a solid thermodynamic basis (Smoller, 1983); being specifically indicated for simulating hyperbolic problems since it preserves shock wave magnitude and position. However Glimm's method implementation requires the complete solution of the associated Riemann problem – a hyperbolic initial value problem subjected to a step function as initial data – once its implementation consists of appropriately gathering the solution of a certain number of associated Riemann problems, whose solution, besides its inherent difficulty, renders the computational implementation more expensive. Non homogeneous hyperbolic systems are conveniently approximated by combining Glimm's method with an operator splitting technique – essentially a technique that treats a simultaneous problem as a sequential one. This procedure has already been successfully used in relevant problems in Mechanics (see Martins-Costa and Saldanha da Gama, 2005 and references therein).

The preliminary hyperbolic model for the transport of pollutants in the atmosphere employed in this work considers the atmosphere an ideal isothermal gas and the pollutants radially transported. It combines the mass and linear momentum balances for the air-pollutant mixture – the classical equations of gas dynamics – with the pollutant mass balance – in which a term representing the rate of pollutants production or destruction due to chemical reactions is considered. The mathematical representation consists of a nonlinear non homogeneous system of hyperbolic partial

* Corresponding author

differential equations presenting discontinuities in addition to classical solutions with a very interesting feature – a contact shock characterized by presenting the same speed of the second eigenvalue. Along this shock the pollutants concentration jump while the mass density and the velocity remain constant, i.e. they do not jump (Martins-Costa and Saldanha da Gama, 2003).

This system numerical simulation is performed by following a systematic procedure consisting of splitting the operator into an ordinary part and a hyperbolic one which, in turn, is treated by means of a Glimm's scheme for evolution in time, employing the Riemann solver proposed by Saldanha da Gama and Martins-Costa (2007) for each two consecutive steps. The use of a Riemann solver allows building a simple and efficient procedure for simulating hyperbolic systems circumventing the requirement of a complete solution for the associated Riemann problem. This solution is approximated by piecewise constant functions satisfying the jump conditions, but not necessarily the entropy condition. The above-mentioned procedure, associated with Glimm's scheme, provides a convenient way for simulating hyperbolic systems. Simulations of transport phenomena in an atmosphere containing *m* pollutants illustrate this above-described methodology. Also, a comparison among results obtained by employing an exact solution of the associated Riemann problem with the proposed Riemann solver results shows the good performance of the latter methodology.

2. MECHANICAL MODEL

A simplified model, based on the mass and linear momentum conservation for the air-pollutants mixture and the mass balances for the *m* pollutants, describes the transport of pollutants in the air. Further assumptions are considering the mass transfer caused by an advection-diffusion process of the pollutants – denoted as A_i constituents – in the air, assumed as an ideal gas. Also supposing the summation of the *m* pollutants (the *i-th* constituents) mass densities negligible compared to the air mass density, the mixture balance equations are approximated by mass and linear momentum balances for the air. Defining ρ as the air mass density, **v** as its velocity, and *p* and **g** as the pressure and specific body force acting on the air, the transport of *m* pollutants in the air is mathematically described as:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \\
&\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) = -\nabla p + \rho \mathbf{g} \\
&\frac{\partial (\rho \omega_i)}{\partial t} + \nabla \cdot (\rho \omega_i \mathbf{v}) = \nabla \cdot (\rho D_i \ \nabla \omega_i) + r_i \qquad i = 1, m
\end{aligned} \tag{1}$$

in which ω_i is the *i-th* constituent concentration (or mass fraction) in the mixture, expressed by $\omega_i \equiv \rho_i / \rho$ where ρ_i is the *i-th* constituent mass density. Diffusion of *m* constituents in the mixture – represented by the coefficients $D_{i,}$ is neglected, when compared to advection, an admissible assumption for an isotropic explosion. A simple constitutive assumption accounting for chemical reactions altering the quantity of the constituents describes the rate of production of the *i-th* constituent: $r_i = -\alpha_i \omega_i$, in which α_i is a constant. At this point it is important to state additional simplifying assumptions to be considered in the present work. First, the pressure acting on the air is considered as a function of the mass density ρ only, its derivative satisfying $\hat{p}'(\rho) > 0$. Also, considering a one-dimensional radial flow, the velocity field may be reduced to a single component on the flow direction $\mathbf{v} = v\mathbf{e}_r$. Besides, gravitational effects will be omitted – a reasonable hypothesis for a radial flow. The above-stated assumptions reduce the mechanical model presented in equation (1) to:

$$\begin{cases}
\dfrac{\partial \rho}{\partial t} + \dfrac{\partial (\rho v)}{\partial r} = -\dfrac{2\rho v}{r} \\
\dfrac{\partial}{\partial t}(\rho v) + \dfrac{\partial}{\partial r}(\rho v^2 + p) = -\dfrac{2\rho v^2}{r} \\
\dfrac{\partial}{\partial t}(\rho \omega_i) + \dfrac{\partial}{\partial r}(\rho \omega_i v) = -\dfrac{2\rho v \omega_i}{r} - \alpha_i \omega_i, \qquad i = 1, m
\end{cases} \tag{2}$$

Defining the following dimensionless quantities: $\eta = r/R,\ \tau = t\breve{v}/R,\ \tilde{\rho} = \rho/\breve{\rho},\ \tilde{v} = v/\breve{v},\ \tilde{p} = p/\breve{\rho}\breve{v}^2$, in which *R* is a reference radius, $\breve{v}$ a reference velocity and $\breve{\rho}$ a reference mass density and considering the redefinition of variables: $F \equiv \tilde{\rho},\ G \equiv \tilde{\rho}\tilde{v},\ H_i \equiv \tilde{\rho}\omega_i$, problem (2) is rewritten as

$$\frac{\partial F}{\partial \tau}+\frac{\partial G}{\partial \eta}=-\frac{2}{r}G$$
$$\frac{\partial G}{\partial \tau}+\frac{\partial}{\partial \eta}\left(\frac{G^2}{F}+\tilde{p}\right)=-\frac{2}{r}\frac{G^2}{F} \tag{3}$$
$$\frac{\partial H_i}{\partial \tau}+\frac{\partial}{\partial \eta}\left(\frac{GH_i}{F}\right)=-\frac{2}{r}\frac{GH_i}{F}-\alpha_i\frac{H_i}{F}\ , \qquad i=1,m$$

It is worth mentioning that in order to solve the above stated problem; initial data for the mass density, the velocity and the pollutants concentration are required. Eventually boundary conditions may also be employed in the solution.

3. NUMERICAL APPROXIMATION

This section presents a scheme to approximate equations (3), based on two main ingredients: an operator splitting technique combined with Glimm's scheme, which in this work is combined with an approximate Riemann solver for advancing in time. The operator splitting consists in decomposing the operator in such a way that its hyperbolic part is splitted away from the purely time evolutionary one. Glimm's method, specifically developed to deal with hyperbolic non-linear problems, consists in marching from a time *n* to a time *n*+1 through the associated Riemann problem for each two consecutive time steps. It is based on a theory whose mathematical formulation has a solid thermodynamic basis, which could be expressed by the entropy condition (Smoller, 1983). A wide range of non-linear hyperbolic problems have already been simulated by combining Glimm's scheme and an operator splitting technique among which are the wave propagation in gas pipelines, shock propagation in gas dynamics problems and wave propagation in a damageable elasto-viscoplastic pipe, the response of non-linear elastic rods and the isothermal and non-isothermal flow of either ideal or Newtonian fluids through unsaturated porous media (see Martins-Costa et al., 2005 and references therein).

Glimm's method approximates the homogeneous part of the hyperbolic operator represented in equation (3), employing the solution of the associated Riemann problem to march from a time *n* to a time *n*+1, thus requiring the solution (or approximation) of the associated Riemann problem. In short, Glimm's method allows building a solution for an initial value problem – namely nonlinear hyperbolic systems subjected to arbitrary initial data, through the solution of a certain number of associated Riemann problems. The initial condition given by a function of the position *r* is approximated by piecewise constant functions, the step functions, with equal width steps. In the sequence a Riemann problem, an initial value problem whose initial condition must be a step function, is to be solved – either exactly or by employing the Riemann solver employed in this work – for each two consecutive steps (Martins-Costa and Saldanha da Gama, 2003). The main idea behind the method is to appropriately gather the solution (or approximation) of as many Riemann problems as desired to successively march from time $\tau=\tau_n$ to time $\tau_{n+1}=\tau_n+\Delta\tau$.

The first step consists in obtaining an initial approximation for (F,G,H_i) by advancing $\Delta\tau$ in time through the homogeneous (merely hyperbolic) part of the operator via Glimm's method, using the values of (F,G,H_i) at time $\tau=\tau_n$ as initial data. The numerical approximation for the solution at time $\tau=\tau_n$ is then obtained by advancing in time with the same time step $\Delta\tau$ through the purely time evolutionary system. This procedure is repeated until reaching a specified simulation time.

The numerical procedure employed to advance from the time $\tau=\tau_n$ to $\tau=\tau_{n+1}$ may be defined as the combination of problem (3) with:

$$F=\hat{F}_n(\eta);\quad G=\hat{G}_n(\eta);\quad H_i=\hat{H}_{i_n}(\eta),\ i=1,m;\quad \text{at } \tau=\tau_n \tag{4}$$

3.1. Operator splitting technique

The fist step to approximate the fields *F*, *G* and H_i at the time $\tau=\tau_{n+1}$ in the non-homogeneous problem described in equations (3)-(4) is to employ an operator splitting technique, described in details by Martins-Costa and Saldanha da Gama (2001). It consists of a decomposition of the operator defined in equation (3) so that its merely hyperbolic part – namely the homogeneous associated system, is split away from its purely time evolutionary one – an ordinary system. This technique gives rise to an initial approximation, obtained by advancing $\Delta\tau$ in time through the equations representing the homogeneous problem, by employing Glimm's method. Once this approximation has been evaluated,

the numerical approximation for the solution (F,G,H_i) at time $\tau = \tau_{n+1}$ is finally reached by advancing in time to solve the following time evolutionary problem, with the same step $\Delta\tau = \tau_{n+1} - \tau_n$ through equations:

$$\left\{\begin{array}{l} \dfrac{\partial F}{\partial \tau} = -\dfrac{2}{\eta} G \\ \dfrac{\partial G}{\partial \tau} = -\dfrac{2}{\eta}\dfrac{G^2}{F} \\ \dfrac{\partial H_i}{\partial \tau} = -\dfrac{2}{\eta}\dfrac{GH_i}{F} - \alpha_i \dfrac{H_i}{F}, \quad i = 1, m \end{array}\right. \qquad \left.\begin{array}{l} F = \hat{F}_{n+1}(\eta) \\ G = \hat{G}_{n+1}(\eta) \\ H_i = \hat{H}_{i_{n+1}}(\eta) \end{array}\right\} \text{ at } \tau = \tau_n \tag{5}$$

with

$$\begin{aligned} F = \hat{F}_{n+1}(\eta) &\approx \tilde{F}_{n+1}(\eta) - \left\{\frac{2}{r}\tilde{G}_{n+1}(\eta)\right\}\Delta\tau \\ G = \hat{G}_{n+1}(\eta) &\approx \tilde{G}_{n+1}(\eta) - \left\{\frac{2}{\eta}\frac{\left[\tilde{G}_{n+1}(\eta)\right]^2}{\tilde{F}_{n+1}(\eta)}\right\}\Delta\tau \\ H_i = \hat{H}_{i_{n+1}}(\eta) &\approx \tilde{H}_{i_{n+1}}(\eta) - \left\{\frac{2}{r}\frac{\tilde{G}_{n+1}(\eta)\tilde{H}_{i_{n+1}}(\eta)}{\tilde{F}_{n+1}(\eta)} + \alpha_i \frac{\tilde{H}_{i_{n+1}}(\eta)}{\tilde{F}_{n+1}(\eta)}\right\}\Delta\tau, \quad i = 1, m \end{aligned} \tag{6}$$

3.2. Glimm's scheme

Glimm's scheme, specifically developed to deal with discontinuous problems, preserves the shock waves magnitude and position, within an uncertainty of $\Delta\eta$ (width of each step). Such features are not found in the usual numerical procedures (e.g. finite elements and finite differences). Besides, Glimm's method presents a clear advantage of saving computer storage memory, when compared to other methodologies such as a finite element method associated with a shock capture procedure, however its limitation to one-dimensional problems is an important shortcoming.

The fields $\tilde{F}_{n+1}(\eta)$, $\tilde{G}_{n+1}(\eta)$ and $\tilde{H}_{i_{n+1}}(\eta)$ used as initial data in (5) are obtained by advancing Δt in time via Glimm's method through the following homogeneous problem:

$$\left\{\begin{array}{l} \dfrac{\partial F}{\partial \tau} + \dfrac{\partial G}{\partial \eta} = 0 \\ \dfrac{\partial G}{\partial \tau} + \dfrac{\partial}{\partial \eta}\left(\dfrac{G^2}{F} + \tilde{p}\right) = 0 \\ \dfrac{\partial H_i}{\partial \tau} + \dfrac{\partial}{\partial \eta}\left(\dfrac{GH_i}{F}\right) = 0, \quad i = 1, m \end{array}\right. \qquad \left.\begin{array}{l} F = \hat{F}_n(\eta) \\ G = \hat{G}_n(\eta) \\ H_i = \hat{H}_{i_n}(\eta) \end{array}\right\} \qquad \text{at } \tau = \tau_n \tag{7}$$

The generalized solution of the Riemann problem associated with the hyperbolic system (7), is reached by connecting the left (L) and right (R) states by means of two intermediate constant states (*1 and *2) as follows: $\left(F_L, G_L, H_{i_L}\right) \rightarrow \left(F_{*1}, G_{*1}, H_{i_{*1}}\right) \rightarrow \left(F_{*2}, G_{*2}, H_{i_{*2}}\right) \rightarrow \left(F_R, G_R, H_{i_R}\right)$. The connection between the states $L \rightarrow *1$, $*1 \rightarrow *2$ and $*2 \rightarrow R$ may be performed either by rarefactions or shocks. A particular type of link is verified in the Riemann problem associated to (7) – the connection between intermediate states *1 and *2 is always a contact shock (Lax, 1971; Smoller, 1983), in which there is no jump for both variables F and G – in such a way that $F_{*1} = F_{*2}$ and $G_{*1} = G_{*2}$. The jump is verified solely for H_i, with a propagation speed G/F. A contact shock may be viewed as the limiting case of a rarefaction in which the rarefaction fan is reduced to a single line; namely a discontinuity with associated eigenvalue corresponding exactly to the shock speed (Martins-Costa and Saldanha da Gama, 2003).

System (7) is approximated by employing Glimm's scheme, described in details in Martins-Costa and Saldanha da Gama (2003), to advance from time τ_n to time τ_{n+1}, in other words, $\tilde{F}_{n+1}(\eta)$, $\tilde{G}_{n+1}(\eta)$ and $\tilde{H}_{i_{n+1}}(\eta)$ are the solutions of (7) evaluated at the time $\tau = \tau_{n+1}$. Glimm's scheme for building a solution for an initial value problem consists in appropriately gathering the solution of a certain previously chosen number of Riemann problems to successively march from time $\tau = \tau_n$ to time $\tau_{n+1} = \tau_n + \Delta\tau$. The arbitrary initial condition given by a function of the position η ($F(\eta,0) = F_0(\eta)$, $G(\eta,0) = G_0(\eta)$, $H_i(\eta,0) = H_{i_0}(\eta)$) is approximated by piecewise constant functions, by convenience, with equal width steps:

$$\left.\begin{aligned} F &= \hat{F}_n(\eta) \approx F_{n_j} = \hat{F}_n(\eta_j + \theta_n \Delta\eta) \\ G &= \hat{G}_n(\eta) \approx G_{n_j} = \hat{G}_n(\eta_j + \theta_n \Delta\eta) \\ H_i &= \hat{H}_{i_n}(\eta) \approx H_{i_{n_j}} = \hat{H}_{i_n}(\eta_j + \theta_n \Delta\eta) \end{aligned}\right\} \quad \text{for} \quad \eta_j - \frac{\Delta\eta}{2} < \eta < \eta_j + \frac{\Delta\eta}{2} \tag{8}$$

in which θ_n is a number randomly chosen in the open interval $(-1/2\,,\ +1/2)$ and $\Delta\eta$ is the width of each step ($\Delta\eta = \eta_{j+1} - \eta_j$).

The above approximations for the initial data give rise, for each two consecutive steps, to the following Riemann problem:

$$\left.\begin{aligned} &\frac{\partial F}{\partial \tau} + \frac{\partial G}{\partial \eta} = 0 \\ &\frac{\partial G}{\partial \tau} + \frac{\partial}{\partial \eta}\left(\frac{G^2}{F} + \tilde{p}(F)\right) = 0 \\ &\frac{\partial H_i}{\partial \tau} + \frac{\partial}{\partial \eta}\left(\frac{G H_i}{F}\right) = 0 \end{aligned}\right\} \quad \begin{cases} (F,G,H) = \left(F_{n_j}, G_{n_j}, H_{i_{n_j}}\right) & \tau = \tau_n\ , -\infty < \eta < \eta_j + \dfrac{\Delta\eta}{2} \\ (F,G,H_i) = \left(F_{n_{j+1}}, G_{n_{j+1}}, H_{i_{n_{j+1}}}\right) & \tau = \tau_n\ ,\ \eta_{j+1} - \dfrac{\Delta\eta}{2} < \eta < \infty \end{cases} \tag{9}$$

Denoting by $F^R_{n_j}$ $G^R_{n_j}$, and $H^R_{i_{n_j}}$ the generalized solution of the Riemann problem (9), the approximation for the solution of (7) at the time $\tau = \tau_{n+1}$ is given as follows:

$$\begin{aligned} F &= \hat{F}_{n+1}(\eta) \approx F^R_{n_j}(\eta, \tau_{n+1}) && \eta_j < \eta < \eta_{j+1} \\ G &= \hat{G}_{n+1}(\eta) \approx G^R_{n_j}(\eta, \tau_{n+1}) && \eta_j < \eta < \eta_{j+1} \\ H_i &= \hat{H}_{i_{n+1}}(\eta) \approx H^R_{i_{n_j}}(\eta, \tau_{n+1}) && \eta_j < \eta < \eta_{j+1} \end{aligned} \tag{10}$$

Remark: In order to prevent interactions among nearby waves of adjacent Riemann problems, the time step $\Delta\tau$ and, consequently, τ_{n+1} for problem (9), must be chosen in such a way that the Courant-Friedrichs-Lewy condition (Smoller, 1983) is satisfied, thus assuring uniqueness for the solution:

$$\tau_{n+1} - \tau_n \le \frac{\Delta\eta}{2|\lambda|_{\max}} \tag{11}$$

4. THE ALTERNATIVE PROCEDURE

The procedure proposed in this work consists in replacing the classical exact solutions of the Riemann problem (9) by generalized approximations – built in by assuming any two given states always connected by a discontinuity which may not satisfy the entropy conditions – in order to advance in time through Glimm's scheme. Essentially the approximation consists in searching for a weak solution for the associated Riemann problem within a space of piecewise constant functions with a maximum of two jumps.

A generalized solution for the Riemann problem described in equations problem (9), depending on (η,τ), may be expressed as a function of a similarity variable $\xi = \eta/\tau$ (Smoller, 1983; Saldanha da Gama, 1990) being constructed by connecting the left (*L*) and right (*R*) states to an intermediate state (*) by rarefactions or shocks as follows: $(F_L, G_L, H_L) \rightarrow (F_*, G_*, H_*) \rightarrow (F_R, G_R, H_R)$ or $(F_L, G_L) \rightarrow (F_*, G_*) \rightarrow (F_R, G_R)$.

Since the connection between intermediate states *1 and *2 in problem (9) is a contact shock – a reversible shock without any associated entropy generation (Saldanha da Gama, 1990) – a continuous solution for problem (9) cannot be reached. This contact shock is characterized by absence of jump for both variables ρ and ρv – in such a way that $(\rho)_{*1} = (\rho)_{*2}$ and $(\rho v)_{*1} = (\rho v)_{*2}$. The jump is verified solely for $\rho\omega_i$, with a propagation speed v ($s_2 = \lambda_2 = v$) – the speed assuming the same value of the corresponding eigenvalue (Martins-Costa and Saldanha da Gama, 2003), giving rise to an important simplification, allowing the former three-variables problem (9) to be reduced to a two variables (v and ρ) one with only two connections to be determined, namely,

$$L \underset{R1 \text{ or } S1}{\Longrightarrow} * \underset{R3 \text{ or } S3}{\Longrightarrow} R \tag{12}$$

in which *R1* and *R3* denote possible rarefaction in connections 1 and 3 while *S1* and *S3* refer to possible shock in these connections.

4.1. On the Riemann solver

It is important to mention that the presence of the contact shock in (9), provides the independent solution of the first two equations of problem (9) as explained by equation (12). The determination of the intermediate state (*) permits solving the third equation. All the considerations above allow expressing the associated Riemann problem as:

$$\left.\begin{aligned} \frac{\partial F}{\partial \tau} + \frac{\partial G}{\partial \eta} &= 0 \\ \frac{\partial G}{\partial \tau} + \frac{\partial}{\partial \eta}\left(\frac{G^2}{F} + \tilde{p}(F)\right) &= 0 \end{aligned}\right\} \quad \tau > \bar{\tau}\,, \qquad -\infty < \eta < \infty$$

$$\begin{aligned} (F,G) &= (F_L, G_R) \qquad \text{for} \quad \tau = \bar{\tau}\,, \quad \eta < \bar{\eta} \\ (F,G) &= (F_R, G_R) \qquad \text{for} \quad \tau = \bar{\tau}\,, \quad \eta > \bar{\eta} \end{aligned} \tag{13}$$

The eigenvalues of (13) are given (in increasing order) by $\lambda_j = G/F + (j-2)(\tilde{p}')^{1/2}$, $j = 1,3$.

Since $\tilde{p}' > 0$ for all η and τ, (13) is hyperbolic system (genuinely nonlinear whenever $\tilde{p}''$ is positive everywhere) and problem (13) is called a Riemann problem whose generalized solution depends on the ratio $(\eta - \bar{\eta})/(\tau - \bar{\tau})$, being reached by connecting the left state (F_L, G_L) and the right state (F_R, G_R) to an intermediate state.

When the eigenvalues λ_j are increasing functions of $(\eta - \bar{\eta})/(\tau - \bar{\tau})$ between two states, they are connected by a *j*-rarefaction (Lax, 1971; John, 1974) – a continuous solution of the associated Riemann problem – the solution (F,G) depending continuously on $(\eta - \bar{\eta})/(\tau - \bar{\tau})$ between these two states and associated to a *j*-rarefaction there exists a Riemann invariant which is a constant. Conversely, if λ_j are decreasing functions, the states are connected by a *j*-shock (a discontinuous solution) with speed s_j, the entropy conditions being automatically satisfied. Since weak solutions cannot assure uniqueness of solution (Keyfitz and Kranzer, 1978), the so-called entropy condition must be verified in order that uniqueness is preserved. Considering two given states connected by a *j*-Shock with speed s_j, the following jump conditions – denoted as Rankine-Hugoniot conditions – associated with equation (13), must be satisfied:

$$s_j = \frac{[\![G]\!]}{[\![F]\!]} = \frac{[\![G^2/F + p]\!]}{[\![G]\!]} \tag{14}$$

in which s_j represents the speed of discontinuity propagation and $[\![f]\!]$, the jump of a quantity *f*.

Details on the employed Riemann solver are found in Saldanha da Gama and Martins-Costa (2007). Essentially it consists of assuming the solution within a space of piecewise constant functions, so that any two states are connected by

a discontinuity. In other words: $(F_L, G_L) \rightarrow$ 1-shock $\rightarrow (F_*, G_*) \rightarrow$ 2-shock $\rightarrow (F_R, G_R)$. This approximation no longer requires considering the original four possible solutions required by Riemann problem exact solution and stated in equation (12). On the other hand, the entropy conditions are not ensured. It is to be noticed that the conservation laws are satisfied in a weak sense.

The (generalized) solution of (13), within a space of piecewise constant functions, is reached as follows ($z = (\eta - \bar{\eta})/(\tau - \bar{\tau})$):

$$(F,G) = \begin{cases} (F_L, G_L) & \text{if} \quad -\infty < z < s_1 \\ (F_*, G_*) & \text{if} \quad s_1 < z < s_2 \\ (F_R, G_R) & \text{if} \quad s_2 < z < \infty \end{cases} \tag{15}$$

5. SOME RESULTS

In order to show the good performance of the Riemann solver proposed in this work, figures 1 to 4 compare results obtained by employing the exact solution of the associated Riemann problem to those using the Riemann solver described in this work. In all depicted sketches, the evolution of gas density ρ, velocity v and pollutants concentration per unit volume for three distinct pollutants – denoted as constituents 1, 2 and 3 of the mixture – namely $\rho\omega_1$, $\rho\omega_2$ and $\rho\omega_3$, is presented along with radial position for five selected time instants. Each considered case is shown in a set composed by six lines and five columns of graphs. Each line represents a distinct time instant – the first one being the initial condition, while each column corresponds to the behavior of a distinct variable. Also, in all depicted graphs, the sphere's internal radius is depicted at the left-hand side while the external one is at the right side. The qualitative results shown in Figures 1 to 4 were obtained by employing a convenient normalization.

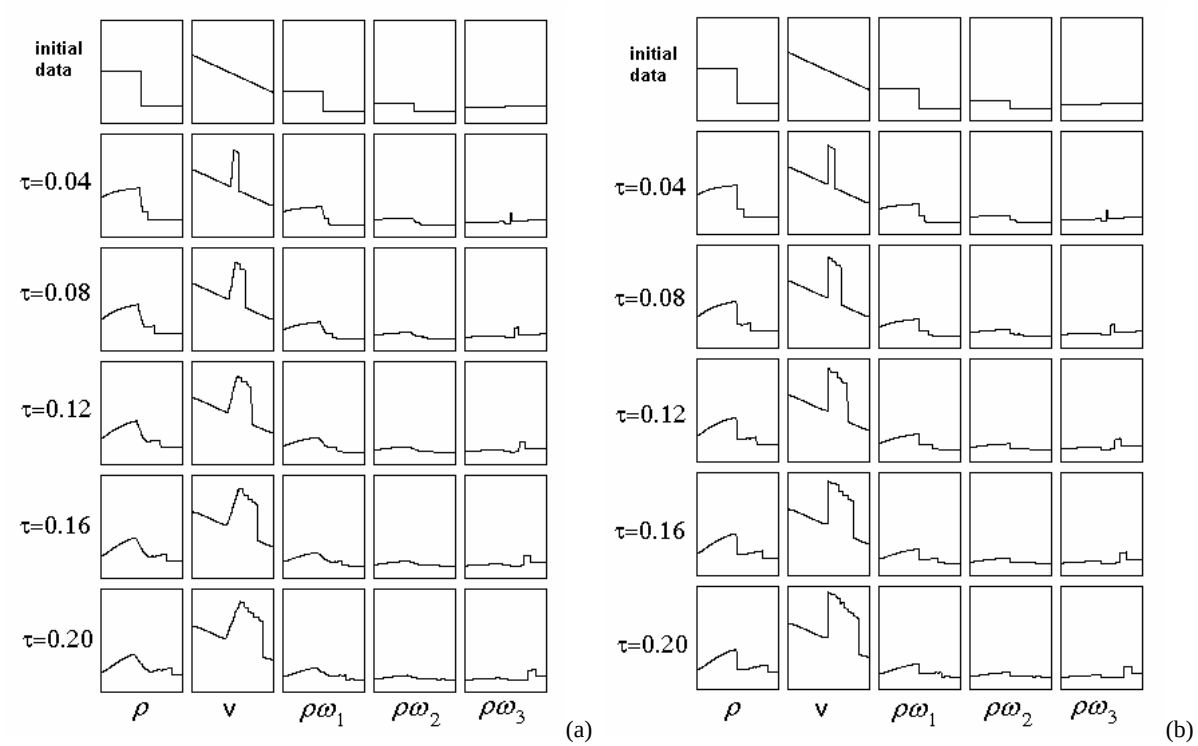

Figure 1. Gas density, velocity and pollutants concentration per unit volume ($\rho\omega_{i(j=1,2,3)}$) variation with radial position for distinct time instants – initial data: step functions for ρ, ω_1, ω_2 and ω_3 and linear velocity. (a) Exact solution of Riemann problem; (b) Riemann solver.

All numerical results have been obtained by employing Glimm's difference scheme combined with an operator splitting technique as described in the previous section employing 200 evolutions in time between each two depicted time instants (except for Figure 1, where 400 evolutions have been considered) while the spatial domain encompassed

300 steps. In all the considered cases the term accounting for rate of production of the constituent 1 was 0.1 ($\alpha_1 = 0.1$) while those related to the constituents 2 and 3 were made equal to zero. Also all results model an isothermal process.

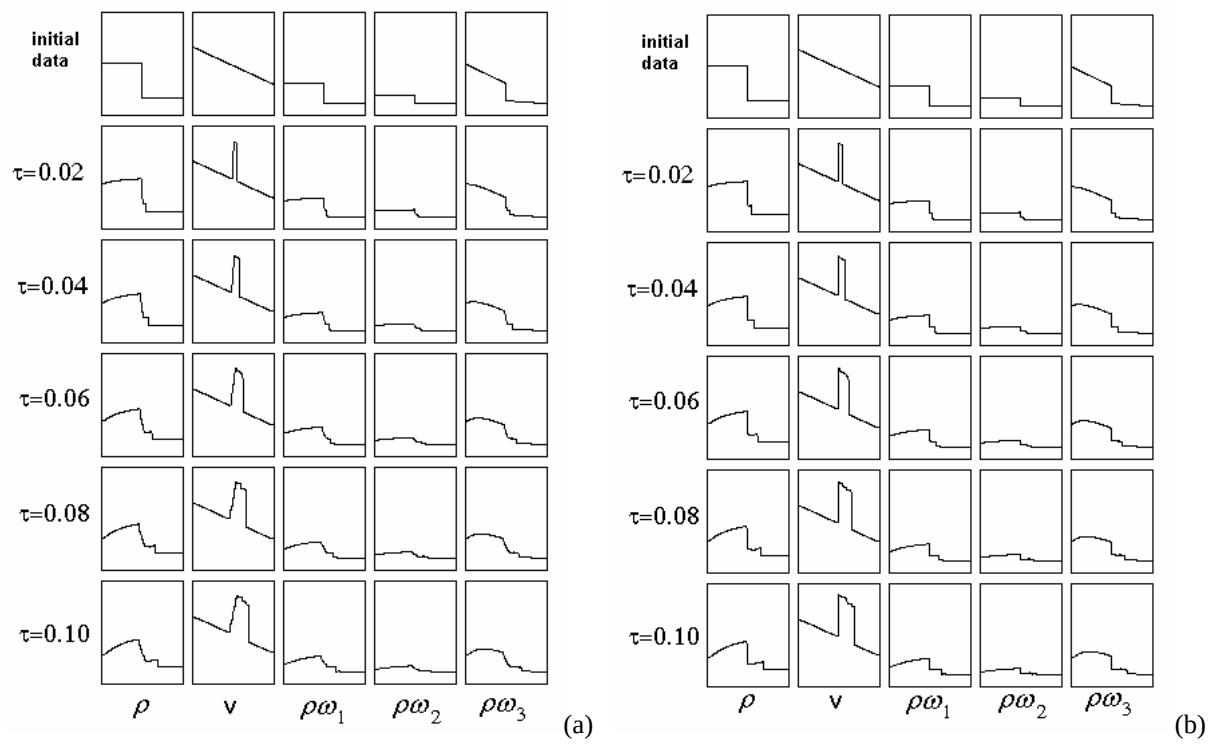

Figure 2. Gas density, velocity and pollutants concentration per unit volume ($\rho\omega_{i(j=1,2,3)}$) variation with radial position for distinct time instants – initial data: step functions for ρ , ω_1 and ω_2 and linear ω_3 and velocity. (a) Exact solution of Riemann problem; (b) Riemann solver.

Figure 1 considers step functions for all the pollutants concentration and for the mass density and a linear decreasing function for the velocity. Figure 2 considers the same initial condition used to obtain Figure 1 except for the third constituent whose pollutants concentration is a linear decreasing function. In Figure 3 step functions were prescribed for the pollutants concentration of the constituents 1 and 2, and a linear decreasing function for the constituent 3 was considered, while the velocity assumed a linear decreasing value up to a region near the spherical shell centerline when it assumes a constant value. Finally in figure 4 step functions were prescribed for all the pollutants concentration and for the velocity while the mass density assumed a linear decreasing function.

At this point it is important to emphasize that in all depicted results both the exact solution of the associated Riemann problem and the Riemann solver proposed by Saldanha da Gama and Martins-Costa (2007) have shown very good agreement, justifying the use of the alternative procedure in the simulation of nonlinear hyperbolic systems.

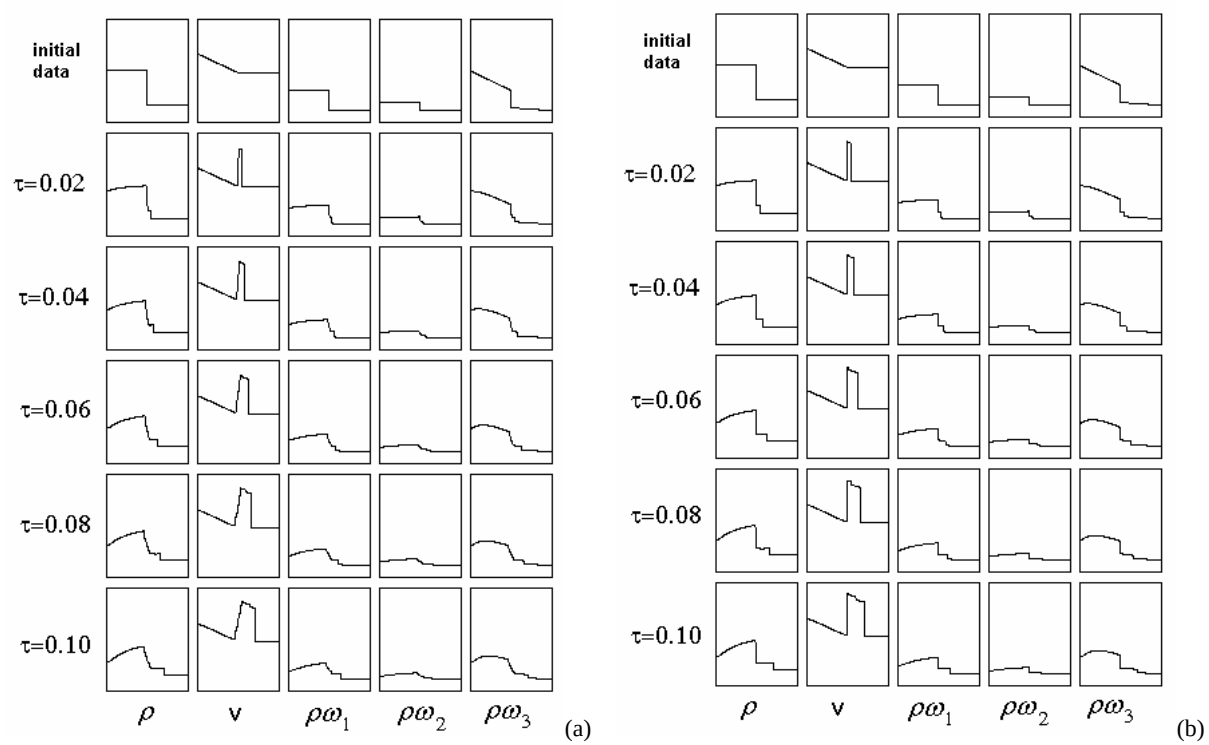

Figure 3. Gas density, velocity and pollutants concentration per unit volume ($\rho\omega_{i(j=1,2,3)}$) variation with radial position for distinct time instants – initial data: step functions for ρ , ω_1 and ω_2 ; linear ω_3 and velocity: linear and constant. (a) Exact solution of Riemann problem; (b) Riemann solver.

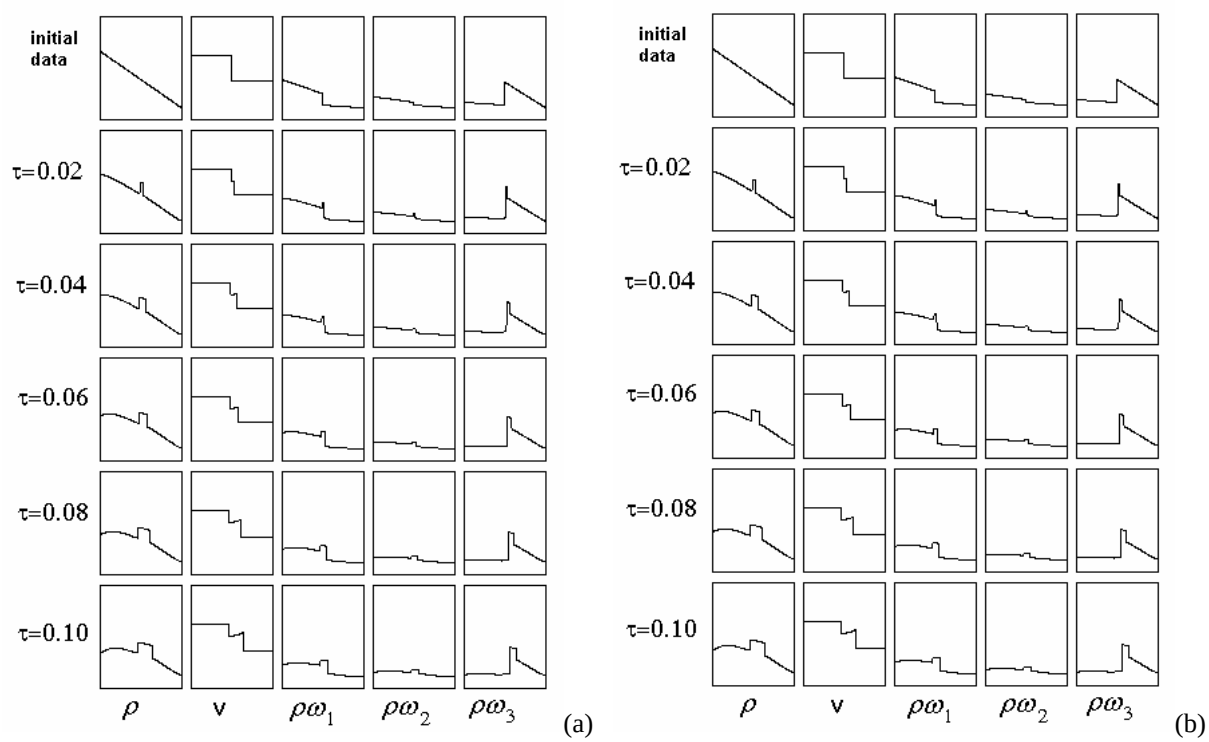

Figure 4. Gas density, velocity and pollutants concentration per unit volume ($\rho\omega_{i(j=1,2,3)}$) variation with radial position for distinct time instants – initial data: step functions for velocity, ω_1 , ω_2 and ω_3 ; and: linear ρ .
(a) Exact solution of Riemann problem; (b) Riemann solver.

6. FINAL REMARKS

The numerical methodology presented in this work allowed the accurate approximation of a nonlinear system of three partial differential equations representing mathematically the transport of n pollutants in the atmosphere. Both the spherical geometry and generation term for one of the pollutants resulted in a nonlinear non homogeneous hyperbolic system, adequately treated by combining Glimm's scheme with operator splitting technique.

Among the numerical methodologies currently employed to treat discontinuous problems Glimm's scheme is the one that better preserves the shock identity. Although its applicability is restricted to one-dimensional problems, this methodology exhibits two important features deserving remark. The former is that Glimm's method approximation tends to the exact solution of the problem (considering its weak formulation) when the width of the steps tends to zero and the latter is that it does not dissipate shocks, preserving their magnitude (no diffusion being observed) and position. The operator splitting technique is a simple and effective tool that consists, essentially, in treating a simultaneous problem as a sequential one. A decomposition in two parts of the operator defined in the hyperbolic system is performed so that the merely hyperbolic part of the operator – namely the homogeneous associated problem – is split away from its purely time evolutionary one.

A Riemann solver was employed to implement Glimm's method for advancing in time. The problem was also approximated by employing the usual methodology for implementing Glimm's scheme – a complete solution of the associated Riemann problem. Comparison between these two solutions has shown very good agreement.

7. ACKNOWLEDGEMENTS

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