SIMULATION OF RADIAL TRANSPORT OF THREE POLLUTANTS IN A NITROGEN ATMOSPHERE

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Abstract. *In this work, the model and simulation of transport phenomena in an environment representing an adiabatic nitrogen atmosphere containing three pollutants is presented. The mathematical model consists of mass and momentum conservation for the nitrogen-pollutant mixture as well as the mass balance for the three pollutants. Some simplifying assumptions give rise to a nonlinear hyperbolic system of five coupled partial differential equations. The problem is solved subjected to a discontinuous initial condition – a jump, originating, in most cases, shock waves. The resulting hyperbolic system is numerically approximated by means of Glimm's scheme, combined with an operator splitting technique to account for the non-homogeneous portion of the hyperbolic operator. Some representative examples illustrate the numerical methodology.*

Keywords: *Pollutants transport, Glimm's scheme, operator splitting.*

1. INTRODUCTION

This work is concerned with model and numerical simulation of three non-reacting pollutants' transport in an environment representing a nitrogen atmosphere. The presence of pollutants in the atmosphere may provoke important effects, justifying the increasing interest devoted to studying transport phenomena in nitrogen -pollutants mixtures. A simplified model, in which the nitrogen is treated as an ideal adiabatic gas, is considered to describe the advection-diffusion transport of the pollutants in the nitrogen. Besides, assuming that the pollutants' mass is negligible with respect to the nitrogen mass, it is possible to obtain a mathematical model consisting of a system of five partial differential equations. These equations are the nitrogen mass and momentum balances and the three mass transport equations – referring to the three pollutants, assuming the diffusion process governed by Fick's law.

The mathematical representation of this phenomenon, considering a one dimensional geometry, consists of a nonlinear system of five partial differential equations, whose unknowns are the

nitrogen density and velocity as well as the three pollutants concentration – all functions of the position x and time t. The problem is solved subjected to a discontinuous initial condition – a jump – originating, in most cases, shock waves.

Modeling of most transport phenomena usually gives rise to parabolic or elliptic partial differential equations. Such mathematical descriptions always admit regular solutions whose simulation may employ well-known numerical procedures such as finite elements, finite differences or finite volumes. Hyperbolic systems, on the other hand, allow very realistic descriptions, since the propagation speed in real natural phenomena is finite. However they may not admit regular solutions – requiring special tools for reliable simulations such as, for instance, Glimm's scheme or Godunov's one. An efficient numerical methodology to simulate these problems would be Glimm's scheme – a numerical method specially designed to deal with problems involving discontinuities and shock waves propagation. This method preserves the shock identity, in other words, the shock waves magnitude and position. When compared to other numerical procedures to approximate nonlinear problems like, for instance, a finite element method associated with a shock capture procedure, Glimm's method exhibits features such as low storage costs and low computational effort, however its limitation to one-dimensional problems is an important shortcoming.

Glimm's methodology is very convenient for dealing with the homogeneous associated problem, which, in this case, is represented by the purely hyperbolic part of the operator. So, an operator splitting technique – essentially a decomposition of the hyperbolic operator in two parts so that the merely hyperbolic part of the operator is split away from its purely time evolutionary one – is combined with Glimm's scheme. More specifically, it consists of advancing in time through the equations representing the homogeneous problem, employing Glimm's method to obtain an initial approximation. Once this approximation has been evaluated, the numerical approximation for the solution at a successive time instant is finally reached by advancing in time to solve the purely time evolutionary problem, employing the same step.

Glimm's scheme, in turn, consists of employing the solution of the associated Riemann problem to generate approximate solutions of the hyperbolic equations, when subject to arbitrary initial data. The main idea behind the method is to appropriately gather the solution of as many Riemann problems as desired to march from a time n to a time n+1. Essentially, every time step of this evolutionary problem is implemented by solving a certain number of associated Riemann problems – one for each two consecutive steps. Representative numerical results for a mixture of nitrogen and three different pollutants – showing the evolution of nitrogen mass density and velocity (approximating the mixture mass density and velocity) as well as the three pollutants concentration – are presented.

2. MECHANICAL MODEL

The transport of three pollutants in a nitrogen atmosphere is described by considering the mass and linear momentum conservation for the nitrogen-pollutants mixture and the mass balance for the pollutants along with some simplifying assumptions. The mass transfer is supposed to be caused by an advection process of the pollutants – from now on denoted as j- constituents – in the nitrogen, which is assumed as an ideal gas (all viscosity effects being neglected), giving rise to:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \\
&\rho \left[\frac{\partial \mathbf{v}}{\partial t} + (\nabla \mathbf{v})\mathbf{v} \right] = \frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) = -\nabla p + \rho \mathbf{g} \\
&\rho \left[\frac{\partial \omega_j}{\partial t} + (\nabla \omega_j) \cdot \mathbf{v} \right] = \frac{\partial (\rho \omega_j)}{\partial t} + \nabla \cdot (\rho \omega_j \mathbf{v}) = \nabla \cdot \mathbf{j}_j + r_j \qquad j = 1,3
\end{aligned} \tag{1}$$

in which ρ stands for the mixture mass density, $\mathbf{v}$ for its velocity, p is the pressure and $\mathbf{g}$ the specific body force (accounting for gravitational effects) acting on the mixture. The concentration of each *j*- constituent in the mixture, being expressed as $\omega_j \equiv \rho_j / \rho$ is defined as the mass fraction of each *j*- constituent in the mixture. Besides, $\mathbf{j}_j$ represents the *j*-constituent mass flux vector and r_j the rate of production of the *j*-constituent. The most important simplifying assumption considered in this work consists in supposing the presence of a sufficiently small quantity of all the three pollutants in the nitrogen – at any time instant. As a consequence, the mass and linear momentum balance equations for the mixture can be approximated by mass and linear momentum balances for the nitrogen. This simplifying assumption allows a convenient redefinition of some variables – ρ is considered as the nitrogen mass density, $\mathbf{v}$ its velocity, and p and $\mathbf{g}$ the pressure and specific body force acting on the nitrogen.

At this point it is important to state additional simplifying assumptions to be considered in the present work. First, the pressure is considered as being a function of the mass density ρ only, its derivative with respect to ρ being given by p' and satisfying $\hat{p}'(\rho) > 0$. Also no chemical reaction, which could alter the quantity of the any of the j constituents with concentration ω_j, will be allowed, leading to $r_j = 0$, for all the five constituents in the mixture. Besides, considering a radial flow in a spherical geometry, the velocity field may be reduced to a single component on the flow direction $\mathbf{v} = v\mathbf{e}_r$ and gravitational effects may be omitted. Finally diffusion may be neglected, when compared to advection – a reasonable one for an isotropic explosion – in other words, $\nabla \cdot \mathbf{j}_j = 0$, $j = 1,3$. All these above mentioned simplifying assumptions give rise to the following nonlinear system of five equations

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial r} = -\frac{2\rho v}{r} \\
&\frac{\partial (\rho v)}{\partial t} + \frac{\partial (\rho v^2)}{\partial r} + p' \frac{\partial \rho}{\partial r} = -\frac{2\rho v^2}{r} \\
&\frac{\partial (\rho \omega_j)}{\partial t} + \frac{\partial (\rho \omega_j v)}{\partial r} = -\frac{2\rho v \omega_j}{r} \qquad j = 1,3
\end{aligned} \tag{2}$$

The present work main subject is to simulate the mechanical problem represented by the non-linear non-homogeneous system of partial differential equations stated in equation (2) subjected to appropriate initial data, which at $t = t_n$, may be represented as $\rho = \hat{\rho}_n(r)$, $v = \hat{v}_n(r)$ and $\omega_j = \hat{\omega}_{j_n}(r)$, $j = 1,3$.

2. NUMERICAL PROCEDURE

This section presents the numerical procedure to simulate system (2) with appropriate initial data. The approximation is carried out by combining Glimm's scheme, which employs in a special way the solution of the associated Riemann problem to advance from a time *n* to a time *n*+1, with an operator splitting technique to account for the non-homogeneous portion of the nonlinear hyperbolic operator. This methodology has already been used with success to approximate distinct nonlinear hyperbolic problems – among which are wave propagation in fluids, wave propagation in a damageable elasto-viscoplastic pipe, gas dynamics problems, the filling-up of a porous matrix, the isothermal and non-isothermal flows of a Newtonian fluid through an unsaturated porous slab and the response of non-linear elastic rods (see Martins-Costa and Saldanha da Gama, 2001 and references therein).

Glimm's method mathematical formulation (Glimm, 1965; Chorin, 1976) is endowed with a solid thermodynamic basis, expressed by the entropy condition, rendering it a convenient numerical methodology to simulate non-linear hyperbolic problems (Martins-Costa and Saldanha da Gama, 2003). The construction of an approximate solution for an initial value problem – namely a nonlinear hyperbolic system subjected to arbitrary initial data – consists in appropriately gathering the solution of a certain number of associated Riemann problems. Consequently, this solution must be known in order to apply Glimm's scheme to a given system. The arbitrary initial condition given by a function of the position r is approximated by piecewise constant 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 for each two consecutive steps. Essentially, Glimm's scheme appropriately assembles the solution of a certain number of Riemann problems (according to a previously settled precision) in order to successively advance from time $t = t_n$ to time $t_{n+1} = t_n + \Delta t$.

At this point, a convenient redefinition of variables, $F \equiv \rho, G \equiv \rho v, H_j \equiv \rho\omega_j$, $j = 1, m$, allows to express problem (3) as:

$$\left.\begin{aligned} &\frac{\partial F}{\partial t} + \frac{\partial G}{\partial r} = -\frac{2G}{r} \\ &\frac{\partial G}{\partial t} + \frac{\partial}{\partial r}\left(\frac{G^2}{F} + p\right) = -\frac{2}{r}\frac{G^2}{F} \\ &\frac{\partial H_i}{\partial t} + \frac{\partial}{\partial r}\left(\frac{GH_i}{F}\right) = -\frac{2}{r}\frac{GH_i}{F} \qquad j = 1,3 \end{aligned}\right\} \qquad \left.\begin{aligned} F &= \hat{F}_n(r) \\ G &= \hat{G}_n(r) \\ H_j &= \hat{H}_{j_n}(r) \end{aligned}\right\} \quad \text{at} \quad t = t_n \qquad (3)$$

in which $F = \hat{F}_n(r,t)$, $G = \hat{G}_n(x,t)$ and $H_j = \hat{H}_{j_n}(r,t)$.

3.1. Operator splitting technique

The first step to approximate the system (3) is to employ an operator splitting technique. The procedure is analogous to the one adopted by Martins-Costa and Saldanha da Gama (2001) to simulate a non-linear non-homogeneous hyperbolic system of two partial differential equations, describing an unsaturated flow through a porous matrix. Basically, the operator presented in equations (3) is decomposed in two problems – namely the homogeneous associated problem (the purely hyperbolic portion) and an ordinary system obtained by considering the purely time evolutionary problem. An initial approximation is obtained by advancing Δt in time through the equations representing the homogeneous problem simulated by Glimm's method.

After performing Glimm's method simulation, the numerical approximation for the solution (ρ, v, ω_j), $j = 1,3$ at time $t = t_{n+1}$ is finally reached by advancing in time – with the same step $\Delta t = t_{n+1} - t_n$ previously employed in Glimm's scheme – to solve the following time evolutionary problem:

$$\left.\begin{aligned} &\frac{\partial F}{\partial t} = -\frac{2G}{r} \\ &\frac{\partial G}{\partial t} = -\frac{2}{r}\frac{G^2}{F} \\ &\frac{\partial H_j}{\partial t} = -\frac{2}{r}\frac{GH_j}{F} \qquad j = 1,3 \end{aligned}\right\} \quad \text{in which} \quad \left.\begin{aligned} F &= \hat{F}_{n+1}(\eta) \\ G &= \hat{G}_{n+1}(\eta) \\ H_j &= \hat{H}_{j_{n+1}}(\eta) \end{aligned}\right\} \quad \text{at} \quad t = t_n \qquad (4)$$

as follows:

$$
\begin{aligned}
F = \tilde{F}_{n+1}(r) &\approx \hat{F}_{n+1}(r) - \left\{ \frac{2G_{n+1}(r)}{r} \right\} \Delta t \\
G = \tilde{G}_{n+1}(r) &\approx \hat{G}_{n+1}(r) - \left\{ \frac{2}{r} \frac{\left[G_{n+1}(r) \right]^2}{F_{n+1}(r)} \right\} \Delta t \\
H_j = \tilde{H}_{j_{n+1}}(r) &\approx \hat{H}_{j_{n+1}}(r) - \left\{ \frac{2}{r} \frac{G_{n+1}(r) H_{j_{n+1}}(r)}{F_{n+1}(r)} \right\} \Delta t \qquad j = 1,3
\end{aligned}
\tag{5}
$$

evaluated at $t = t_{n+1}$ and considering $\Delta t = t_{n+1} - t_n$.

3.2. Glimm's method

An initial approximation for the fields F, G and H_j $(j = 1,3)$ at time t_{n+1}, denoted as $\tilde{F}_{n+1}$, $\tilde{G}_{n+1}$ and $\tilde{H}_{j_{n+1}}$ is obtained by employing Glimm's method in the homogeneous associated problem to equations (4) defined as:

$$
\begin{aligned}
&\frac{\partial F}{\partial t} + \frac{\partial G}{\partial r} = 0 \\
&\frac{\partial G}{\partial t} + \frac{\partial}{\partial r}\left(\frac{G^2}{F} + p \right) = 0 \\
&\frac{\partial H_j}{\partial t} + \frac{\partial}{\partial r}\left(\frac{G H_j}{F} \right) = 0 \qquad j = 1,3
\end{aligned}
\qquad \text{with} \qquad
\begin{aligned}
F &= \hat{F}_n(r) \\
G &= \hat{G}_n(r) \\
H_j &= \hat{H}_{j_n}(r)
\end{aligned}
\qquad \text{at} \qquad t = t_n
\tag{6}
$$

In order to build a solution for the initial value problem presented in equations (6), namely a nonlinear hyperbolic system subjected to arbitrary initial data, the solution of the associated Riemann problem – discussed in details in Martins-Costa and Saldanha da Gama (2003) – must be known. Essentially, Glimm's method consists in performing time evolutions employing the solution of the associated Riemann problem between each two consecutive steps in the spatial discretization.

Initially the arbitrary initial condition given by a function of the position r – in other words: $F(r,0) = F_0(r)$, $G(r,0) = G_0(r)$ and $H_j(r,0) = H_{j_0}(r)$ – is approximated by piecewise constant functions, since the initial condition of each Riemann problem must be a step function. In the present work, these functions have been chosen with equal width steps, by convenience. At a given time t_i this approximation may be expressed as

$$
\begin{aligned}
F = F_n(r) &\approx F_{n_i} = \hat{F}_n(r_i + \theta_n \Delta r) \\
G = G_n(r) &\approx G_{n_i} = \hat{G}_n(r_i + \theta_n \Delta r) \\
H_j = H_{j_n}(r) &\approx H_{j_{n_i}} = \hat{H}_{j_n}(r_i + \theta_n \Delta r) \quad j = 1,3
\end{aligned}
\qquad \text{for} \qquad r_i - \frac{\Delta r}{2} < r < r_i + \frac{\Delta r}{2}
\tag{7}
$$

in which θ_n is a number randomly chosen in the open interval $(-1/2,\ +1/2)$ and Δr is the width of each step ($\Delta r = r_{i+1} - r_i$).

Since the first derivative of the pressure with respect to the mass density, p', is positive, the system presented in equation (3) is a hyperbolic one. When the approximations for the initial data

presented in equation (7) are combined with equation (6) they give rise, for each two consecutive steps, to a Riemann problem (Lax, 1971; Smoller, 1983) associated with equations (6).

The following proceeding consists in solving – for each two consecutive steps – the associated Riemann problem in order to successively march from time $t = t_n$ to time $t_{n+1} = t_n + \Delta t$. This problem is defined as:

$$\begin{aligned} &\frac{\partial F}{\partial t} + \frac{\partial G}{\partial r} = 0 \\ &\frac{\partial G}{\partial t} + \frac{\partial}{\partial r}\left(\frac{G^2}{F} + p\right) = 0 \\ &\frac{\partial H_j}{\partial t} + \frac{\partial}{\partial r}\left(\frac{GH_j}{F}\right) = 0 \qquad j = 1,3 \end{aligned} \tag{8}$$

with

$$\begin{aligned} &\left(F, G, H_j\right) = \left(F_{n_i}, G_{n_i}, H_{j_{n_i}}\right) \qquad \text{for} \quad t = t_n \;,\; -\infty < r < r_i \;,\; j = 1,3 \\ &\left(F, G, H_j\right) = \left(F_{n_{i+1}}, G_{n_{i+1}}, H_{j_{n_{i+1}}}\right) \qquad \text{for} \quad t = t_n \;,\; r_i < r < \infty \;,\; j = 1,3 \end{aligned} \tag{9}$$

Denoting by $\overline{F}_{n_i}$, $\overline{G}_{n_i}$ and $\overline{H}_{n_i}$ the generalized solution of equations (8)-(9), the approximation for the solution of equations (6) at time t_{n+1} is given as follows:

$$\begin{aligned} &F = \hat{F}_{n+1}(r) \approx \overline{F}_{n_i}(r,\, t_{n+1}) \\ &G = \hat{G}_{n+1}(r) \approx \overline{G}_{n_i}(r,\, t_{n+1}) \qquad \text{for} \qquad r_i < r < r_{i+1} \\ &H_j = \hat{H}_{j_{n+1}}(r) \approx \overline{H}_{j_{n_i}}(r,\, t_{n+1}) \quad j = 1,3 \end{aligned} \tag{10}$$

In order to prevent interactions among nearby shocks of adjacent Riemann problems, the time step Δt and, consequently, t_{n+1} must be chosen in such a way that the Courant-Friedrichs-Lewy condition (John, 1982) be satisfied, thus assuring uniqueness for the solution:

$$t_{n+1} - t_n \le \frac{\Delta r}{2\left|\lambda\right|_{\max}} \tag{11}$$

where $\left|\lambda\right|_{\max}$ is the maximum (in absolute value) propagation speed of shocks, considering all the Riemann problems at time t_n. Respecting the CFL condition stated in equation (11), when selecting the time step ensures Glimm's method robustness

At this point it is important to stress some features of Glimm's method, regarding its accuracy. First if the width of the steps tends to zero the approximation obtained by Glimm's method tends to the exact solution of the problem considering its weak formulation. Another characteristic of Glimm's scheme is that it preserves shock magnitude (no diffusion being observed) and position – whose admissible deviation from the correct position is of the order of magnitude of the width of each step. It is also worth mentioning that when compared to other numerical methodologies to approximate nonlinear problems, Glimm's scheme requires both lower storage costs and lower computational effort. However, two important shortcomings of this methodology should be

considered – first its applicability being restricted to one-dimensional problems. Also, its implementation requires previous knowledge of the solution of the associated Riemann problem.

After each advance in time, the obtained solution is no longer given as a step function. Thus a new random selection is required in order to build the initial condition as a step function to perform the time evolution from a given time instant t_n to the next instant t_{n+1} by employing Glimm's method. Once the solution for a given time instant t_n is known, the initial data for the next step, t_{n+1}, is approximated as

$$\begin{aligned} F_{i_n} &= F\left(r_i + \theta_n \Delta r, t_n\right) \\ G_{i_n} &= G\left(r_i + \theta_n \Delta r, t_n\right) \qquad \text{for} \qquad r_i - \frac{\Delta r}{2} < r < r_i + \frac{\Delta r}{2} \\ H_{j_{i_n}} &= H_j\left(r_i + \theta_n \Delta r, t_n\right) \quad j = 1,3 \end{aligned} \tag{12}$$

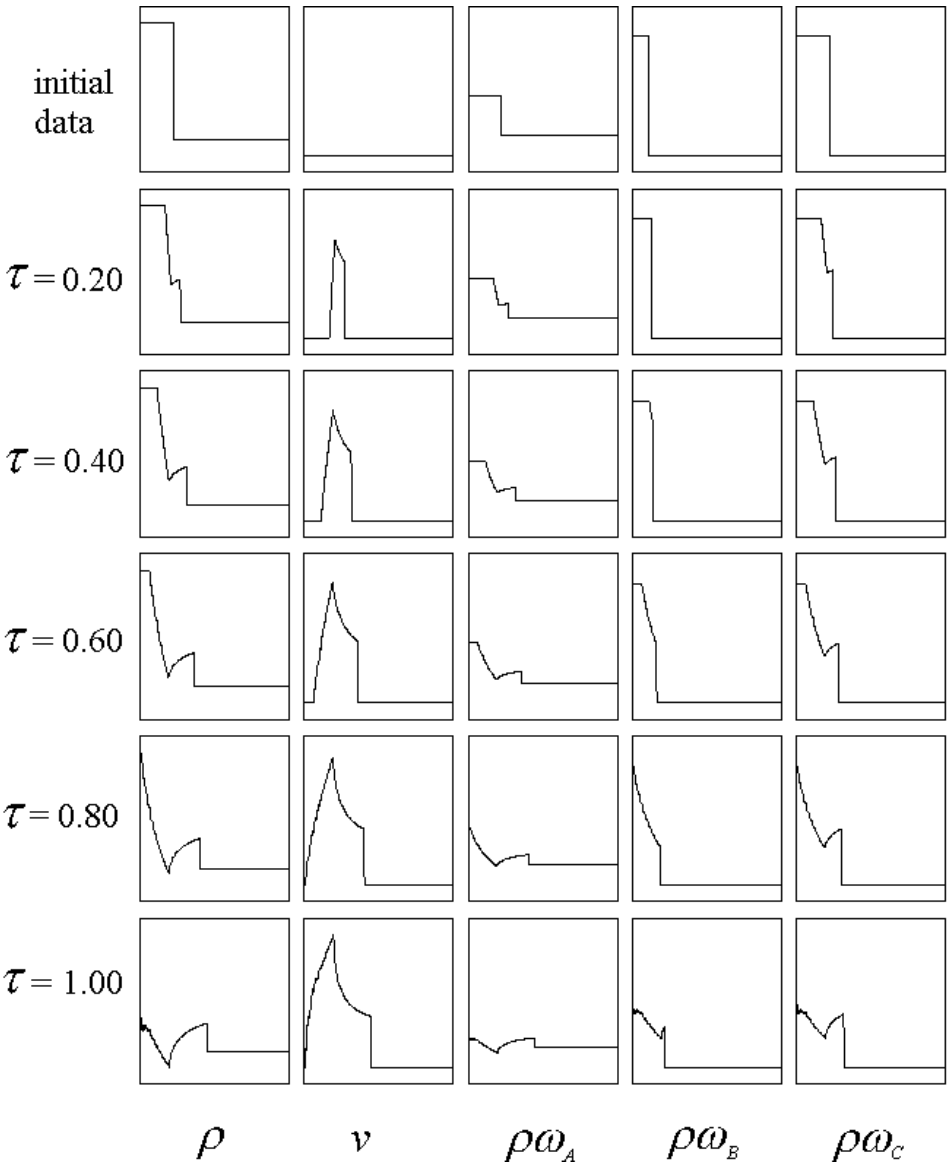

Figure 1. Gas density, velocity and pollutants concentration per unit volume ($\rho\omega_{j(j=A,B,C)}$) variation with radial position – internal radius 0.2 and initial data: step functions for ρ, ω_B and ω_C, zero v and constant ω_A.

4. NUMERICAL RESULTS.

In order to validate the numerical strategy presented in the previous item, figures 1 and 2 show, in all depicted sketches, the evolution of gas density ρ, velocity v and pollutants concentration per unit volume for three distinct pollutants – denoted by A, B and C constituents of the mixture – namely $\rho\omega_A$, $\rho\omega_B$ and $\rho\omega_C$, along with radial position for five selected time instants. Each considered case is presented 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. All the qualitative results shown were obtained by employing a convenient normalization.

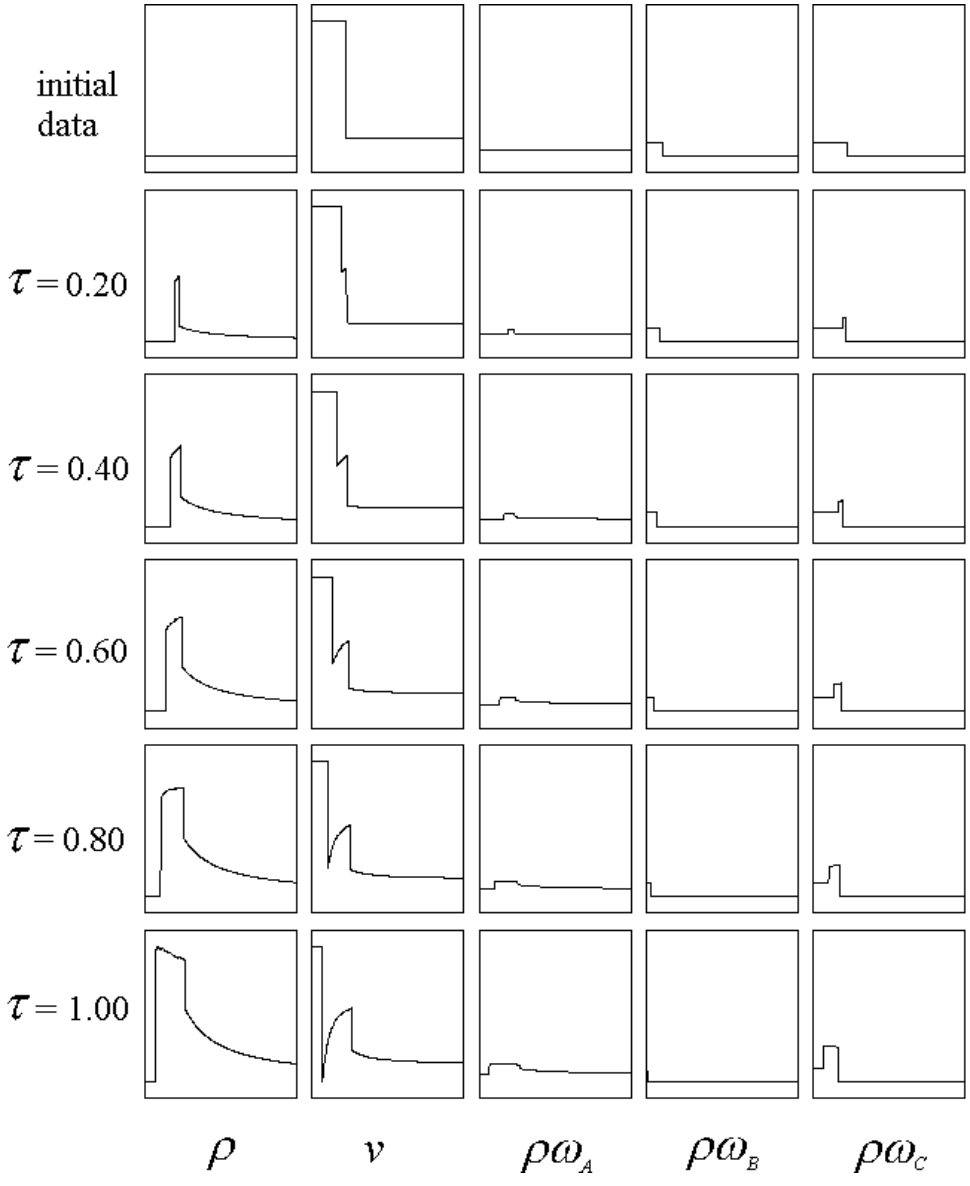

Figure 2. Gas density, velocity and pollutants concentration per unit volume ($\rho\omega_{j(j=A,B,C)}$) variation with radial position – internal radius 0.05 and initial data: step functions for v, ω_B and ω_C, and constant ρ and ω_A.

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 10^4 evolutions in time while the spatial domain encompassed 900 steps. In order to exclude edge effects or, in other words, to assure that the external edge is not reached by a shock or a rarefaction wave – allowing simulating transport phenomena in an infinite environment – the results are shown for a domain including only the 450 internal steps. Also, an impermeable wall is considered by assuming zero velocity at the internal radius. Figure 1 was obtained by considering an internal radius 0.2 while in figure 2 it has been made four times smaller (r_i=0.05), both spherical regions with the same thickness.

Figure 1 employed as initial data step functions for the mass density (jumping from $\rho = 0.9$ at a given region with width δ near the spherical core to $\rho = 0.3$) and for the concentration of the pollutants *B* (jumping from $\omega_B = 1.0$ at an internal region of width $\delta / 2$ to $\omega_B = 0$) and *C* (jumping from $\omega_C = 1.0$ at the region δ to $\omega_C = 0$), zero velocity and a constant value for concentration of the pollutant *A* ($\omega_A = 0.5$). Aiming to simulate an isotropic explosion – in which the pollutants *B* and *C* with distinct distributions are initially confined in a spherical core, while the pollutant *A* is present in the whole domain, it may be observed a flow from left-side to right-side, generated by differences in density.

In all the time instants depicted in figure 1, discontinuities for mass density and velocity at the same spatial position may be observed. This behavior, as expected, is also followed by $\rho\omega_A$, since a constant value has been assumed for ω_A, but not by $\rho\omega_B$ or $\rho\omega_C$. In the velocity profiles evolution a negative inclination after its peak values is observed. This decay effect has been accentuated due to the employed splitting technique.

The initial data employed to generate figure 2 encompasses the same initial values employed in the previous figure for the three pollutants as well as constant mass density ($\rho = 0.1$) and a step function for the velocity (jumping from $v = 0$ at the internal region δ to $v = -0.5$ outside δ). This problem simulates external perturbation acting in the sense of compressing the fluids towards a spherical core, giving rise to a flow from right to left-hand side. This compression effect originates a peak in the mass density. Similarly to figure 1, discontinuities for mass density, velocity and *A*-pollutant concentration at the same spatial position are present in all the time instants depicted in figure 2.

At this point it is important to emphasize that Glimm's scheme – combined with an operator splitting technique, to account for the non-homogeneous part of the differential equations – has already been successfully employed to simulate many nonlinear hyperbolic problems. Examples are wave propagation in fluids (Sod, 1977), gas dynamics problems (Marchesin and Paes-Leme, 1983), the filling-up of a porous matrix (Saldanha da Gama and Sampaio, 1987), the wave propagation in a damageable elasto-viscoplastic pipe (Freitas-Rachid et al. 1994), the response of non-linear elastic rods (Saldanha da Gama, 1990), the non-isothermal flow of a Newtonian fluid through an unsaturated porous matrix (Saldanha da Gama and Martins-Costa, 1997) and the unsaturated flow of a Newtonian fluid through a porous slab – covering most one-dimensional cases of interest (Martins-Costa and Saldanha da Gama, 2001).

Regarding its accuracy, Glimm's method is free from numerical dissipation – preserving shock waves magnitude and presenting a deviation from the correct position smaller than the width of each step – preserving shock waves position. Besides, if the width of the steps tends to zero, Glimm's approximation tends to the exact solution of the problem.

4. FINAL REMARKS

Glimm's method, besides preserving shock waves magnitude and position, is a convenient tool for solving one-dimensional nonlinear problems, exhibiting features such as low storage costs and low computational effort, when compared to other numerical procedures to approximate nonlinear

problems. In order to simulate a nonlinear and non-homogeneous system of hyperbolic equations, Glimm's scheme has been combined with an operator splitting technique – decomposing the operator in a purely time evolutionary part and a merely hyperbolic one – to account for the non-homogeneous portion of the operator.

The numerical methodology presented in this work allowed an accurate approximation of a hyperbolic system of five partial differential equations representing mathematically the transport of three pollutants in a nitrogen atmosphere. An analogous procedure allows taking into account additional effects not considered in this work such as diffusion of the pollutants in the nitrogen atmosphere, pollutants generation (due to chemical reactions, for instance) as well as gravitational effects.

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