NUMERICAL SIMULATION OF NON-REACTING POLLUTANTS TRANSPORT IN AN ADIABATIC ATMOSPHERE

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

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

Abstract. *In this work the model and simulation of transport phenomena in an environment representing an adiabatic atmosphere containing m pollutants is presented. The mathematical model consists of mass and momentum conservation for the air-pollutant mixture as well as the mass balance for the m pollutants. Some simplifying assumptions give rise to a nonlinear hyperbolic system of m+2 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. Some examples considering m=3 illustrate the numerical methodology.*

Keywords*. Non-reacting pollutants transport, shock waves, Glimm difference scheme, Riemann problem.*

1. Introduction

This work is concerned with model and numerical simulation of *m* non-reacting pollutants' transport in an environment representing an adiabatic atmosphere. The presence of pollutants in the atmosphere may provoke important effects, justifying the increasing interest devoted to studying transport phenomena in air-pollutants mixtures. A simplified model, in which the atmosphere is treated as an ideal adiabatic gas, is considered to describe the advection-diffusion transport of the pollutants in the air. Besides, assuming that the pollutants' mass is negligible with respect to the air mass, it is possible to obtain a mathematical model consisting of a system of *m*+2 partial differential equations. These equations are the air mass and momentum balances and the *m* mass transport equations – referring to the *m* 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 with 2 hyperbolic and *m* parabolic partial differential equations, whose unknowns are the air density and velocity as well as the *m* 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.

The resulting system is numerically approximated by means of Glimm difference scheme – a numerical method specially designed to deal with discontinuous problems, which 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. It consists of a numerical procedure 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. In order to employ this scheme the initial data must be approximated by piecewise constant functions giving rise, for each two consecutive steps, to an initial value problem known as the Riemann problem, which must be solved for these two consecutive steps. Essentially, every time step of this evolutionary problem is implemented by solving the a certain number of associated Riemann problems – one for each two consecutive steps. Representative numerical results for a mixture of air and three different pollutants – showing the evolution of air mass density and velocity (approximating the mixture mass density and velocity) as well as the three pollutants concentration – are presented.

2. Mechanical modeling

The transport of *m* pollutants in the air is described by considering the mass and linear momentum conservation for the air-pollutants mixture and the mass balance for each of the *m* 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 air, which is assumed as an ideal gas (all viscosity effects being neglected), giving rise to:

‡ All article correspondence should be addressed to this author.

$$\frac{\partial r}{\partial t}+\nabla\cdot(r\,\mathbf{v})=0$$
$$r\left[\frac{\partial \mathbf{v}}{\partial t}+(\nabla\mathbf{v})\mathbf{v}\right]=\frac{\partial(r\,\mathbf{v})}{\partial t}+\nabla\cdot(r\,\mathbf{vv})=-\nabla p+r\,\mathbf{g} \qquad (1)$$
$$r\left[\frac{\partial w_j}{\partial t}+(\nabla w_j)\cdot\mathbf{v}\right]=\frac{\partial(r w_j)}{\partial t}+\nabla\cdot(r w_j\mathbf{v})=\nabla\cdot\mathbf{j}_j+r_j \qquad j=1,m$$

in which r 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, w_j, is defined as the mass fraction of the *j*-constituent in the mixture, being expressed as $w_j \equiv r_j / r$. 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 *m* pollutants in the air – 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 air. This simplifying assumption allows a convenient redefinition of some variables – r is considered as the air mass density, $\mathbf{v}$ its velocity, and p and $\mathbf{g}$ the pressure and specific body force acting on the air.

Additional simplifying assumptions are now stated: First, the pressure is assumed to be a function of the mass density r only, $p=\hat{p}(r)$, its derivative with respect to r being given by p' and satisfying $\hat{p}'(r)>0$. Second, supposing a plane flow, the velocity field may be reduced to a single component on the flow direction $\mathbf{v}=v\mathbf{i}$. Also no chemical reaction which could alter the quantity of the any of the *j* constituents with concentration w_j will be allowed, leading to $r_j=0$, for all the *m* constituents in the mixture. Finally, two additional hypotheses are considered: a horizontal flow is assumed, allowing to omit gravitational effects and diffusion effects – accounted for in the first term at the right hand side of the third equation of (1) – may be neglected. All these above mentioned simplifying assumptions give rise to the following nonlinear system of *m*+2 equations

$$\frac{\partial r}{\partial t}+\frac{\partial}{\partial x}(r v)=0$$
$$\frac{\partial}{\partial t}(r v)+\frac{\partial}{\partial x}(r v^2+p)=0 \qquad (2)$$
$$\frac{\partial}{\partial t}(r w_j)+\frac{\partial}{\partial x}(r w_j v)=0 \qquad j=1,m$$

3. Numerical methodology

In this section the numerical simulation of system (2) combined with appropriate initial data is presented. The approximation is carried out by using a convenient method: 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. Glimm's method mathematical formulation is endowed with a solid thermodynamic basis, expressed by the entropy condition, rendering it a convenient numerical methodology to simulate non-linear hyperbolic problems.

This methodology, which may be combined with an operator splitting technique to account for the non-homogeneous portion of the nonlinear hyperbolic operator, has already been used with success to approximate distinct nonlinear hyperbolic problems. Among these problems 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). It is remarkable that the problems addressed in these works, due to their hyperbolic nature, do not require boundary conditions, being essentially initial value problems (John, 1982).

Glimm's method approximate solution construction for an initial value problem – namely a nonlinear hyperbolic system subjected to arbitrary initial data – consists in appropriately gather 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 *x* 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 $t_{n+1}=t_n+\Delta t$.

3.1. The associated Riemann problem

The Riemann problem (Smoller, 1983) associated with Eq. (2) must satisfy two conditions: the former requires the system (2) to be a genuinely non-linear hyperbolic one, being assured whenever the first derivative of the pressure with respect to the density, p', is positive. The latter condition is that the problem must be homogeneous in order to remain homogeneous as the dependence on both variables x and t is converted in a dependence on the similarity variable x. Essentially, Riemann problem is a special kind of initial data problem defined as:

$$\frac{\partial}{\partial t}\begin{bmatrix} r \\ rv \\ rw_j \end{bmatrix} + \begin{bmatrix} 0 & 1 & 0 \\ -v^2 + p' & 2v & 0 \\ -vw_j & w_j & v \end{bmatrix} \frac{\partial}{\partial x}\begin{bmatrix} r \\ rv \\ rw_j \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad \text{for } -\infty < x < +\infty,\ t > 0,\ j = 1, m \tag{3}$$

$$\begin{aligned} \left(r, rv, rw_j\right) &= \left((r)_L, (rv)_L, (rw_j)_L\right) \qquad \text{for } x < 0 \quad \text{and} \quad t = 0,\ j = 1, m \\ \left(r, rv, rw_j\right) &= \left((r)_R, (rv)_R, (rw_j)_R\right) \qquad \text{for } x > 0 \quad \text{and} \quad t = 0,\ j = 1, m \end{aligned} \tag{4}$$

In the above stated problem the variables r, v and w_j $(j = 1, m)$ are functions of both *x* and *t*, being subject to a step function as initial condition – specified in Eq. (4), where $\left((r)_L, (rv)_L, (rw_j)_L\right)$ represent its value at the left-hand side and $\left((r)_R, (rv)_R, (rw_j)_R\right)$ its value at the right-hand side.

A problem depending on the set of variables (x,t) may be converted in a problem depending solely on a similarity variable $x = x/t$ provided that two necessary and sufficient conditions are satisfied. First the dependence on x requires constant values for the function both at the left-hand side and at the right-hand side, so that the initial condition must be a step function. This condition allows recovering left-hand side and right-hand side constant values of the initial condition if the characteristic tends to ∞. The second condition is that the problem must be homogeneous in order to remain homogeneous as the dependence on both variables x and t is converted in a dependence on the similarity variable x. Substituting $x = x/t$, the associated Riemann problem may be rewritten as

$$-x\frac{d}{dx}\begin{bmatrix} r \\ rv \\ rw_j \end{bmatrix} + \begin{bmatrix} 0 & 1 & 0 \\ -v^2 + p' & 2v & 0 \\ -vw_j & w_j & v \end{bmatrix} \frac{d}{dx}\begin{bmatrix} r \\ rv \\ rw_j \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad \text{for } -\infty < x < +\infty,\quad j = 1, m \tag{5}$$

$$\begin{aligned} \left(r, rv, rw_j\right) &= \left((r)_L, (rv)_L, (rw_j)_L\right) \qquad \text{for } x \to -\infty,\quad j = 1, m \\ \left(r, rv, rw_j\right) &= \left((r)_R, (rv)_R, (rw_j)_R\right) \qquad \text{for } x \to +\infty,\quad j = 1, m \end{aligned} \tag{6}$$

Glimm's difference scheme (Chorin, 1976) simulates the advective transport of *m* pollutants in the atmosphere – mathematically represented by Eq. (2) by employing the generalized solution of Eqs. (5)-(6). In order to obtain this solution Riemann invariants must be known. This, in turn, requires the determination of the following eigenvalues – in crescent order, corresponding to Eq. (5),

$$l_i = v + a_i\sqrt{p'}, \qquad \text{with} \quad a_i = i - 2 \tag{7}$$

Since the model used in this work requires p' to be an always positive quantity (for all values of x and t) then the system presented in Eq. (5) is a genuinely nonlinear hyperbolic one, the set of Eqs. (5)-(6) being called a Riemann problem. The generalized solution of this Riemann problem depends only on the ratio $x = x/t$ being reached by connecting the left state $\left((r)_L, (rv)_L, (rw_j)_L\right)$ and the right state $\left((r)_R, (rv)_R, (rw_j)_R\right)$ by means of two intermediate states, namely $\left((r)_{*1}, (rv)_{*1}, (rw_j)_{*1}\right)$ and $\left((r)_{*2}, (rv)_{*2}, (rw_j)_{*2}\right)$ as follows: $\left((r)_L, (rv)_L, (rw_j)_L\right)$ $\to$ $\left((r)_{*1}, (rv)_{*1}, (rw_j)_{*1}\right)$ $\to$ $\left((r)_{*2}, (rv)_{*2}, (rw_j)_{*2}\right)$ $\to$ $\left((r)_R, (rv)_R, (rw_j)_R\right)$, in which *1 and *2 indicate intermediate constant states to be determined. Riemann problem solution construction must determine whether the connections between the states $L \to *1$, $*1 \to *2$ and $*2 \to R$ are performed either by rarefactions or shocks. This determination is based on the behavior of the corresponding eigenvalues l_i. If they represent increasing functions of $x = x/t$ between two given states, then these states are connected by an *i*- Rarefaction: a continuous solution of the

Riemann problem. In this case, the solution depends continuously on x between these states. On the other hand, if the eigenvalues l_i are non-increasing functions of $x = x/t$, the states are connected by a discontinuous solution, which may be an *i*-Shock.

Besides these above mentioned connection types, there is also another kind of link – namely a limit-case of rarefaction: a contact shock (Smoller, 1983). In this connection the rarefaction fan is reduced to a single line; namely a discontinuity with associated eigenvalue corresponding exactly to the shock speed. Unlike ordinary shocks, the contact shock is reversible, without any associated entropy generation. This particular type of link occurs between the intermediate states *1 and *2 in the problem (5)-(6). It is characterized by absence of jump for both variables r and rv – in such a way that $(r)_{*1} = (r)_{*2}$ and $(rv)_{*1} = (rv)_{*2}$. The jump is verified solely for rw_j $(j = 1, m)$, with a propagation speed v – the speed assuming the same value of the corresponding eigenvalue.

In order to verify whether the discontinuous solution is a shock, it is required that both the Rankine-Hugoniot jump condition and the entropy condition (Smoller, 1983) be fulfilled . Two states are connected by an *i*-Shock provided that $v + a_i\sqrt{p'}$ is a decreasing function of $x = x/t$. In this case, the entropy condition is automatically satisfied. Considering two given states connected by an *i*-Shock with speed s, the following jump condition – denoted as Rankine-Hugoniot condition, associated with Eq. (5) must be satisfied

$$s = \frac{[\![rv]\!]}{[\![r]\!]} = \frac{[\![rv^2 + p]\!]}{[\![rv]\!]} = \frac{[\![rvw_j]\!]}{[\![rw_j]\!]} \quad , \qquad j = 1, m \tag{8}$$

in which s represents the shock speed and $[\![f]\!]$, the jump of the quantity f.

A remarkable feature of the equality $l = x/t$ is that it is valid only in the presence of a rarefaction fan. Besides, the eigenvalue problem only makes sense in rarefaction regions. When two given states cannot be connected by a continuous solution, one must search for a weak solution, the natural candidates for this weak solution being functions with jump conditions satisfying the Rankine-Hugoniot condition stated in Eq. (8).

It is important to keep in mind that weak solutions cannot assure uniqueness of solution. An additional condition must be verified in order that uniqueness is preserved – the so-called entropy condition, originated from gas dynamics problems (Smoller, 1983), indicating that the entropy of the correct solution must be increased as the solution crosses a shock. The entropy conditions – in the particular case of the Riemann problem presented in Eqs. (5-6) – are given by:

$$l_{1*} < s_1 < l_{1L} \quad \text{and} \quad s_1 < l_{2R} \qquad \text{for the 1–shock,} \tag{9}$$

$$l_{1L} < s_2 = l_{2*} < l_{3R} \qquad \text{for the 2 (contact)–shock and} \tag{10}$$

$$l_{3R} < s_3 < l_{3*} \quad \text{and} \quad l_{2*} < s_3 \qquad \text{for the 3–shock.} \tag{11}$$

It is remarkable that the entropy condition presented in Eq. (10) – representing a contact shock – is, actually, a limit case of entropy condition.

Considering the Riemann problem expressed by Eqs. (5)-(6) two given states are connected by an *i*-shock with speed s_i provided that the jump condition expressed by Eq. (8) is satisfied and the associated eigenvalue is a non increasing function of $x = x/t$ – this latter condition being equivalent to the entropy condition for the class of problems treated in Eqs. (5)-(6). In other words, whenever $r_* > r_L$ the states 1 and * will be connected by a 1-shock (instead of a 1-rarefaction) while * and 2 will be connected by a 3-shock (instead of a 3-rarefaction) whenever $r_R < r_*$.

In short, when two states are connected by a shock, with speed s_i, the jump conditions (8) associated with the Riemann problem stated in Eqs. (5)-(6) must be satisfied.

3.2. Glimm's scheme

At this point a redefinition of variables is performed in order to express the system (2) in a more convenient way:

$$F \equiv r \;, \quad G \equiv rv \;, \quad H_j \equiv rw_j \;, \quad j = 1, m \tag{12}$$

The above redefinition allows to express the complete problem – formed by Eq. (2) and suitable initial data – as

$$\begin{aligned}
&\frac{\partial F}{\partial t}+\frac{\partial G}{\partial x}=0\\
&\frac{\partial G}{\partial t}+\frac{\partial}{\partial x}\left(\frac{G^2}{F}+p\right)=0\\
&\frac{\partial H_j}{\partial t}+\frac{\partial}{\partial x}\left(\frac{GH_j}{F}\right)=0 \qquad j=1,m
\end{aligned} \tag{13}$$

$$\left.\begin{aligned}
F&=\hat{F}_n(x)\\
G&=\hat{G}_n(x)\\
H_j&=\hat{H}_{j_n}(x)
\end{aligned}\right\} \quad \text{at} \quad t=t_n \quad \text{for} \quad j=1,m \tag{14}$$

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

The first step consists in obtaining an initial approximation for (F,G,H_j) by advancing Δt in time via Glimm's method, using the values of (F,G,H_j) at time $t=t_n$ as initial data. In order to apply Glimm's method to build a solution to Eq. (13) subjected to the arbitrary initial data expressed in (14) these data must be approximated by piecewise constant functions. The following piecewise constant functions with equal width steps will be employed in this work:

$$\begin{aligned}
&F=\hat{F}_n(x)\approx F_{n_i}=\hat{F}_n(x_i+q_n\Delta x)\\
&G=\hat{G}_n(x)\approx G_{n_i}=\hat{G}_n(x_i+q_n\Delta x)\\
&H_j=\hat{H}_{j_n}(x)\approx H_{j_{n_i}}=\hat{H}_{j_n}(x_i+q_n\Delta x) \qquad j=1,m
\end{aligned} \tag{15}$$

for $x_i-\frac{\Delta x}{2}<x<x_i+\frac{\Delta x}{2}$, in which q_n is a number randomly chosen in the open interval $(-1/2,\ +1/2)$ and Δx is the width of each step ($\Delta x=x_{i+1}-x_i$).

The associated Riemann problem may be redefined as the combination of Eq. (13) with the following initial conditions:

$$\begin{aligned}
&(F,G,H_j)=\left(F_{n_i},G_{n_i},H_{j_{n_i}}\right) \quad \text{for} \quad -\infty<x<x_i+\frac{\Delta x}{2};\quad t=t_n \quad \text{and} \quad j=1,m\\
&(F,G,H_j)=\left(F_{n_{i+1}},G_{n_{i+1}},H_{j_{n_{i+1}}}\right) \quad \text{for} \quad x_i+\frac{\Delta x}{2}<x<\infty;\quad t=t_n \quad \text{and} \quad j=1,m
\end{aligned} \tag{16}$$

Denoting by $\bar{F}_{n_i},\bar{G}_{n_i}$ and $\bar{H}_{j_{n_i}}$ the generalized solution of Eqs. (13)-(16), the approximation for the solution of Eqs. (13)-(14) at a time instant t_{n+1} is given as follows:

$$\begin{aligned}
&F=\hat{F}_{n+1}(x)\approx\bar{F}_{n_i}(x,\ t_{n+1}) \qquad \text{for} \quad x_i<x<x_{i+1}\\
&G=\hat{G}_{n+1}(x)\approx\bar{G}_{n_i}(x,\ t_{n+1}) \qquad \text{for} \quad x_i<x<x_{i+1}\\
&H_j=\hat{H}_{j_{n+1}}(x)\approx\bar{H}_{j_{n_i}}(x,\ t_{n+1}) \quad \text{for} \quad x_i<x<x_{i+1} \qquad \text{and} \quad j=1,m
\end{aligned} \tag{17}$$

In order to prevent interactions among nearby shocks of adjacent Riemann problems, the Courant-Friedrichs-Lewy condition (John, 1982) must be satisfied, thus assuring uniqueness for the solution. So, the time step Δt must fulfill:

$$t_{n+1}-t_n\le\frac{\Delta x}{2|l|_{\max}} \tag{18}$$

where $|l|_{\max}$ is the maximum (in absolute value) propagation speed of shocks, considering all the Riemann problems at time t_n.

At this point it is important to stress some features of Glimm's method. 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.

After each advance in time, the obtained solution is no longer given as a piecewise constant function. Thus a new random selection is required in order to build the initial condition as a piecewise constant 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 taken as

$$\begin{aligned} F_{i_n} &= F\left(x_i + q_n \Delta x, t_n\right) \\ G_{i_n} &= G\left(x_i + q_n \Delta x, t_n\right) \\ H_{j\,i_n} &= H_j\left(x_i + q_n \Delta x, t_n\right) \quad j = 1, m \end{aligned} \tag{19}$$

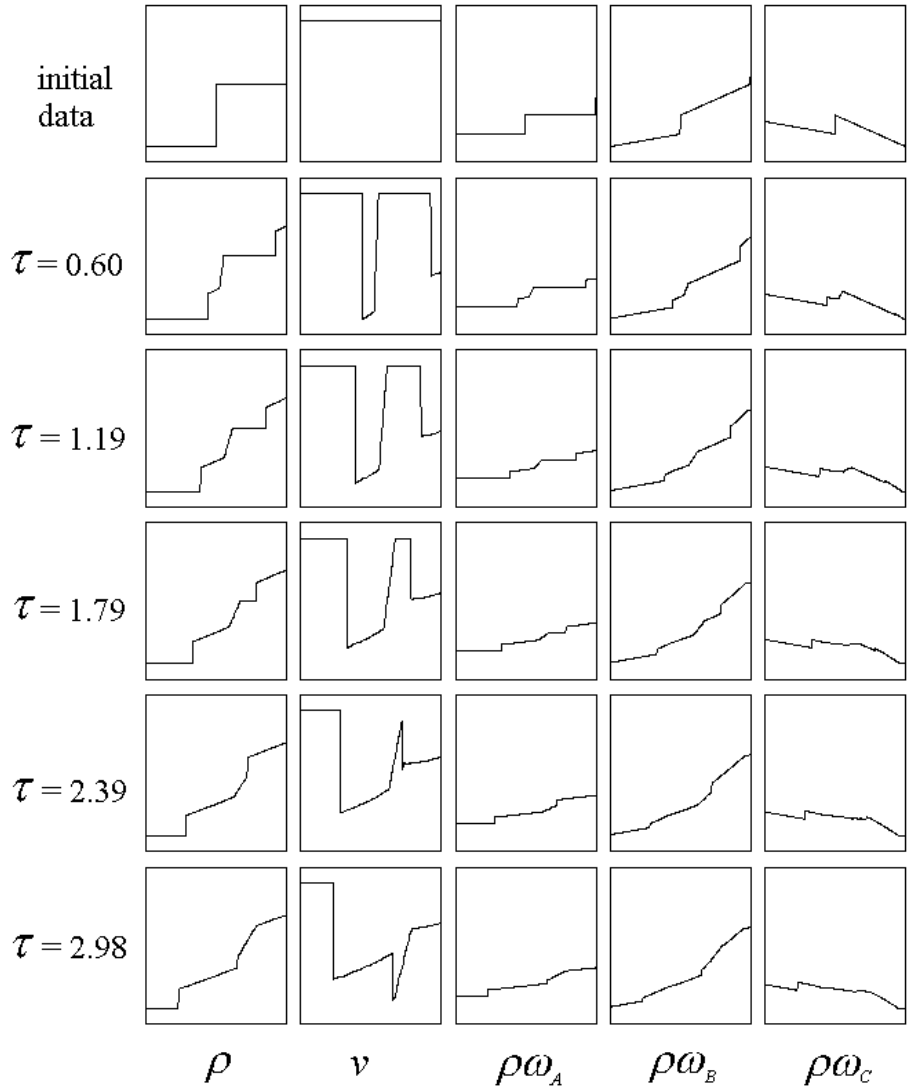

Figure 1. Gas density, velocity and pollutants concentration per unit volume ($rw_{j(j=A,B,C)}$) variation with position initial data: step functions for r , zero v, constant w_A, and distinct linear functions for w_B and w_C .

4. Results

Figures 1 to 4 show – in all depicted sketches, the evolution of gas density r, velocity v and pollutant concentration per unit volume for three distinct pollutants – denoted by *A*, *B* and *C* constituents of the mixture – namely rw_A, rw_B and rw_C, along with 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. All the qualitative results shown were obtained by employing a convenient normalization, in such a way that the minimum and maximum displayed values correspond to zero and unit values for r, v and $rw_{j(j=A,B,C)}$. All numerical results have been obtained by employing Glimm's difference scheme as described in the previous section employing 2500 evolutions in time. Each sketch presents the results for a given vicinity (150 steps of width Δx) of the origin – located at the center of the abscissa – characterizing an infinite environment, while the edges were not reached by a shock or a rarefaction wave.

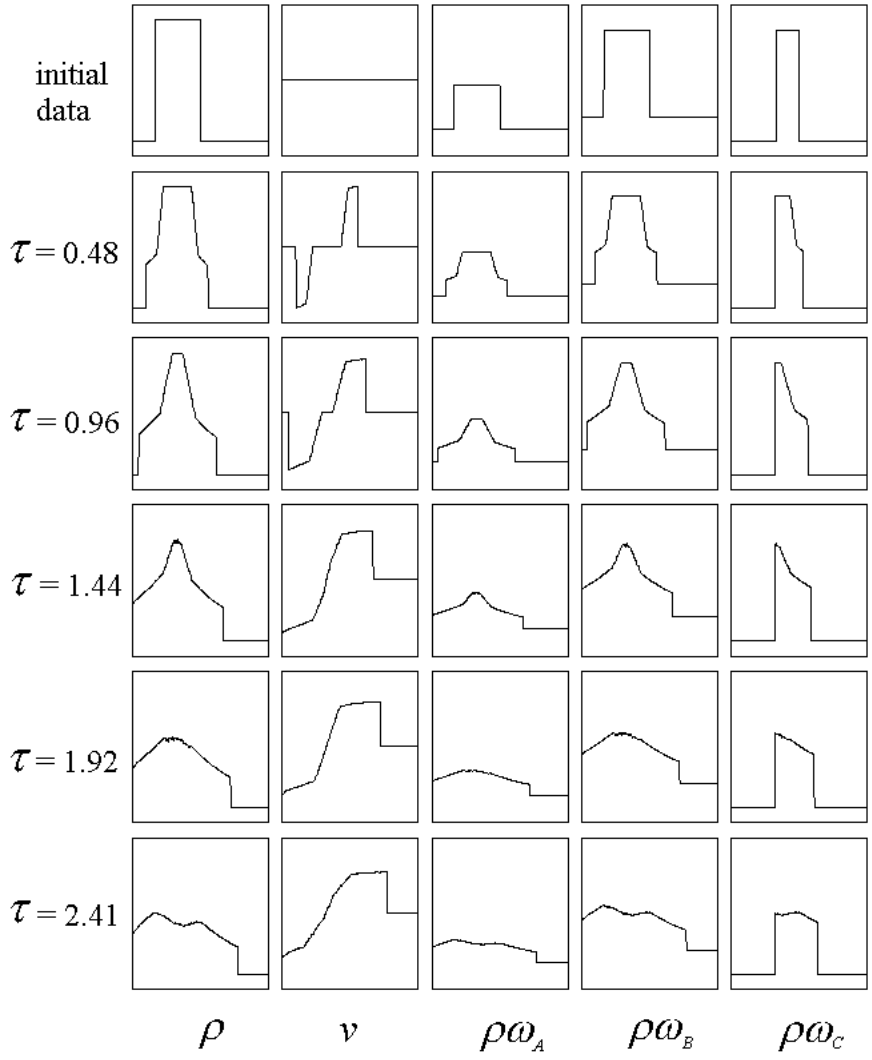

Figure 2. Gas density, velocity and pollutants concentration per unit volume ($rw_{j(j=A,B,C)}$) variation with position
initial data: jumps for r, zero v, constant w_A and w_B and jumps for w_C.

In order to validate the numerical strategy presented in the previous item, the depicted results have been obtained by considering distinct combinations of initial conditions. The variables have been alternatively assumed as constants, step functions, constant in most of the domain – except for an internal region characterized by discontinuities corresponding to one or more higher or lower values. Besides, they also may be given by linear increasing or decreasing functions or by sinusoidal or co-sinusoidal functions.

Figure 1 employed as initial data a step function for the mass density (jumping from $r_L = 0.2$ to $r_R = 0.3$), zero velocity, a constant value for concentration of the pollutant *A* ($w_{A_0} = 0.5$) and linear functions for the concentration of the pollutants *B* (increasing w_B) and *C* (decreasing w_C). It is remarkable that in all the results considered in this work the initial data – depicted in the first line of every figure – show results for the pollutant concentration per unit volume (rw_A, rw_B and rw_C). In Fig. 1 it may be noticed that the discontinuities for the gas density r and gas velocity v (and, consequently, for rw_A, rw_B and rw_C) are located at the same spatial position.

Figure 2 has been obtained by considering as initial data: jumps for r (ranging from $r_0 = 0.2$ to a higher density region characterized by $r_0 = 0.92$), zero velocity, constant values for the concentration of the pollutants *A* and *B* (with w_A = 0.5 and w_B = 1.0) and jumps for the concentration of the pollutant *C* (given by w_C = 1 in a small vicinity of a given point and w_C = 0, otherwise). In all the time instants depicted in Fig. 2, discontinuities for mass density and velocity at the same spatial position may be observed. This behavior, as expected, is also followed by both rw_A and rw_B, but not by rw_C.

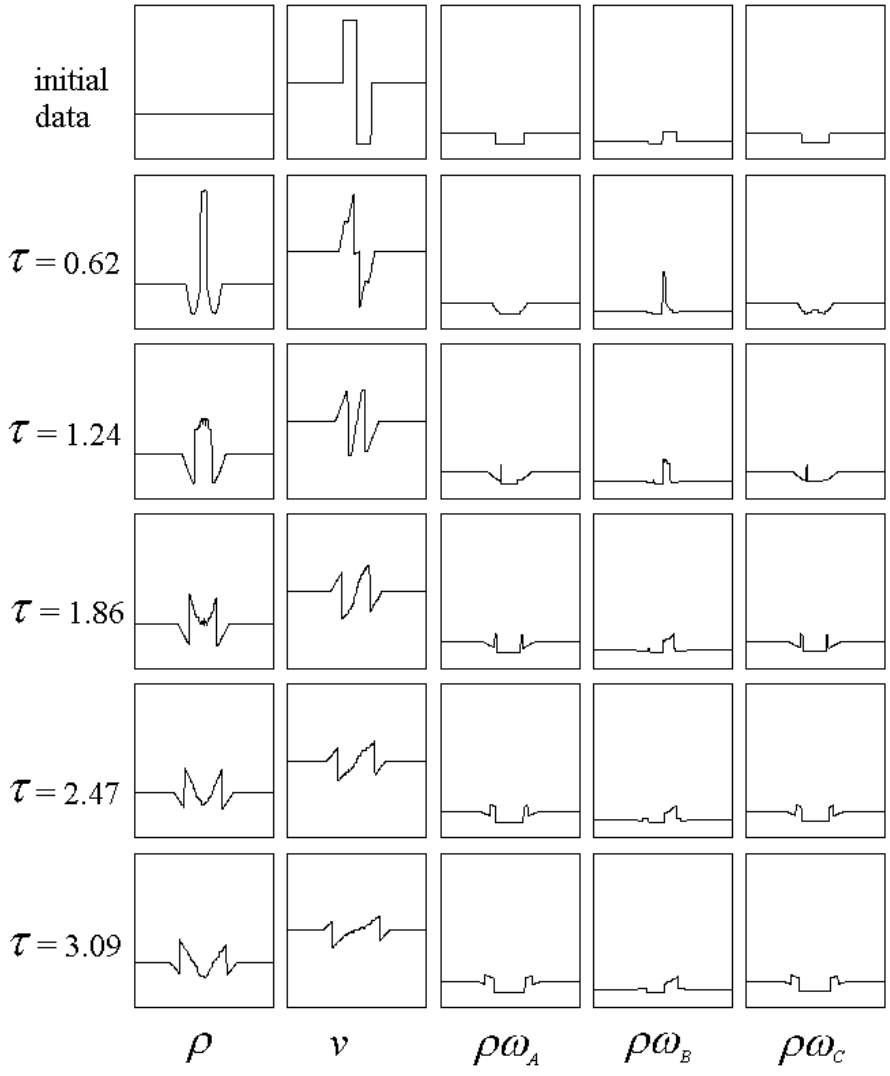

Figure 3. Gas density, velocity and pollutants concentration per unit volume ($rw_{j(j=A,B,C)}$) variation with position
initial data: constant r and distinct jumps imposed on v, w_A, w_B and w_C.

In Fig. 3 a constant mass density (r = 0.1) has been assumed as initial value, the velocity is zero in most of the considered domain – jumping from v = 0.9 to v = – 0.9 at a central region and the pollutants concentration also present

jumps, ranging from one constant value employed in almost the whole domain to another one at a small region, given, respectively, by the sets: $w_A = 0.9$ and $w_A = 0$, $w_B = 0.2$ and $w_B = 1$ and $w_C = 0.9$ and $w_C = 0.1$. In this case, only mass density and velocity present discontinuities at the same spatial position, for every considered t .

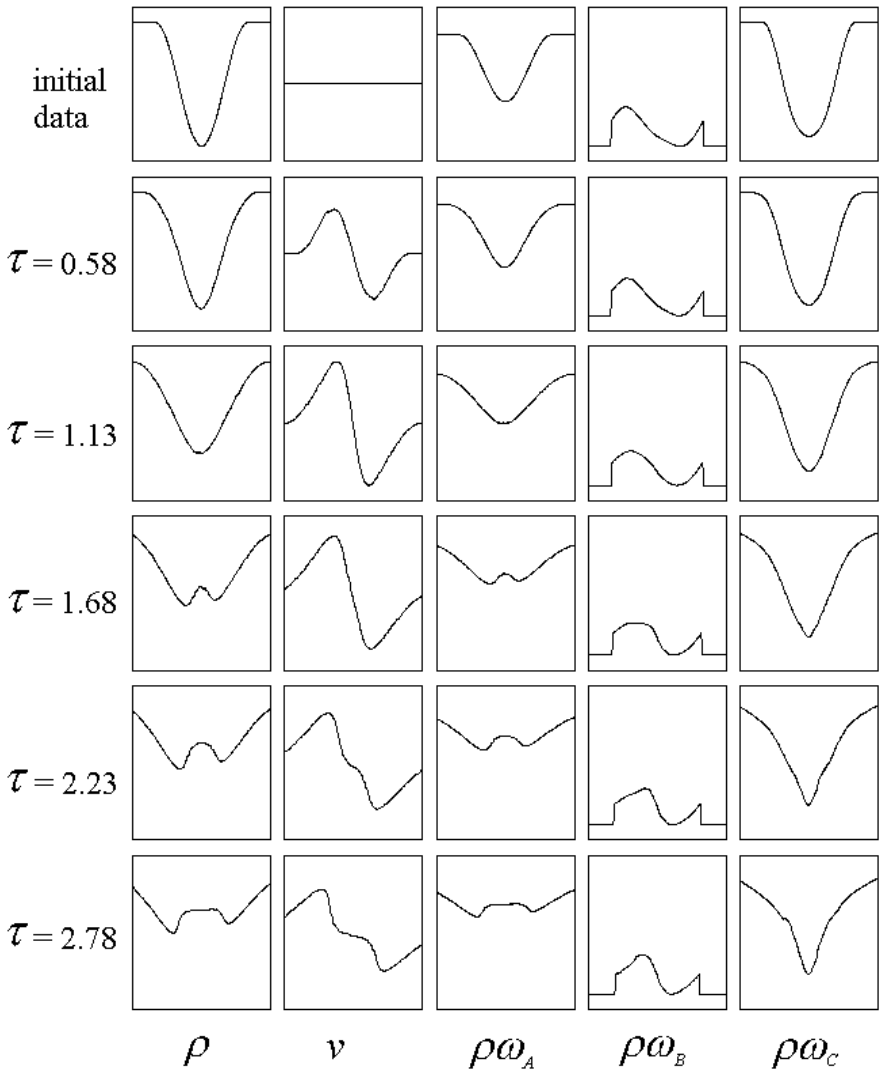

Figure 4. Gas density, velocity and pollutants concentration per unit volume ($rw_{j(j=A,B,C)}$) variation with position initial data: co-sinusoidal functions for r and w_C , sinusoidal function for w_B , constant w_A and zero v .

Figure 4 was obtained by using as initial data distinct co-sinusoidal functions for the mass density r and the concentration of the constituent *C*, w_C , a sinusoidal function for the concentration of the constituent *B*, w_B , a constant value for the concentration of the constituent *A* (w_A = 0.9) and zero velocity. No sharp discontinuities are verified, except for the parameter rw_B – whose initial value is built by combining a sinusoidal function with a co-sinusoidal one.

5. 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.

The numerical methodology presented in this work allowed the accurate approximation of a nonlinear system of m+2 partial differential equations representing mathematically the transport of m pollutants in the atmosphere. Additional effects not considered in this work such as diffusion of the pollutants in the atmosphere, pollutants generation as well as gravitational effects could be accounted for by employing an operator splitting technique (see Martins-Costa and Saldanha da Gama, 2001 and references therein).

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