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RADIAL ADVECTIVE TRANSPORT OF A POLLUTANT IN AN ATMOSPHERE

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Abstract. *A preliminary hyperbolic model is used to describe the transport phenomena in an environment representing an atmosphere containing a pollutant, in which the atmosphere is modeled as an ideal polytropic gas, the is pollutant transported radially and the rate of pollutant production or destruction due to chemical reactions is accounted for. The resulting mathematical description consists of a nonlinear hyperbolic system of three partial differential equations representing mass and momentum conservation for the air-pollutant mixture and the pollutant mass balance. This system simulation is performed by combining Glimm's scheme (whose implementation requires the solution of a Riemann problem for each two consecutive steps) and an operator splitting technique to deal with the non-homogeneous part of the hyperbolic operator, accounting not only for terms arising from the problem spherical geometry but also for the rate of production or destruction of the pollutant.*

Keywords*. Pollutant radial transport, pollutant generation, Glimm's scheme, operator splitting technique.*

1. Introduction

This work employs a preliminary hyperbolic model to describe transport phenomena in an environment representing the atmosphere containing a pollutant. The atmosphere is modeled as an ideal polytropic gas and the pollutant is transported radially. The resulting mathematical representation of this phenomenon consists of a nonlinear hyperbolic system of three partial differential equations representing mass and momentum conservation for the air-pollutant mixture and the pollutant mass balance – in which a term representing the rate of pollutant production or destruction due to chemical reactions is considered.

The nature of this mathematical problem does not allow, in general, classical solutions, in which the differential equations are verified at every spatial point, thus requiring an enlargement of the admissible solutions space, in order to allow for the presence of discontinuities satisfying a certain solution criterion – given by the entropy condition, besides satisfying a weak formulation of the conservation equations.

This system hyperbolic feature suggests its approximation by means of a numerical method specially designed to deal with discontinuous problems. Its simulation is performed by following a systematic procedure consisting of three distinct steps – namely the construction of a Glimm's scheme for time evolution with arbitrary initial condition, the complete generalized solution of the associated Riemann problem (since Glimm's scheme implementation requires, for every time step, the solution of a Riemann problem for each two consecutive steps) and an operator splitting into a hyperbolic part and an ordinary one.

Glimm's scheme is a numerical methodology to treat discontinuous problems, preserving the shock waves magnitude and position. Although its applicability is restricted to one-dimensional problems, this methodology exhibits features such as low storage costs and low computational effort, when compared to other numerical procedures to approximate nonlinear problems. 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.

2. Mechanical model

The transport of a pollutant in the air is described by considering the mass and linear momentum conservation for the air-pollutant mixture and the mass balance for the pollutant along with some simplifying assumptions. First the mass transfer is supposed to be caused by an advection-diffusion process of the pollutant – from now on denoted as *A* constituent, in the air, which is assumed as an ideal gas (all viscosity effects being neglected). The most important

simplifying assumption is to suppose the presence of a sufficiently small quantity of the constituent *A* in the mixture – at any time instant, so that 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 to define ρ as the air mass density, $\mathbf{v}$ as its velocity, and p and $\mathbf{g}$ as the pressure and specific body force acting on the air.

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \\
&\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) = -\nabla p + \rho \mathbf{g} \\
&\frac{\partial (\rho \omega_A)}{\partial t} + \nabla \cdot (\rho \omega_A \mathbf{v}) = \nabla \cdot (\rho D \, \nabla \omega_A) + r_A
\end{aligned} \tag{1}$$

The concentration of the constituent *A* in the mixture, ω_A, is defined as the mass fraction of this constituent in the mixture, being expressed by the following equation $\omega_A \equiv \rho_A / \rho$. Besides, D represents the diffusion coefficient of the constituent *A* in the mixture and r_A the rate of production of the constituent *A*. 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, $p = \hat{p}(\rho)$ its derivative with respect to ρ being given by p' and satisfying $p'(\rho) > 0$. 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 and, finally, diffusion may be neglected, when compared to advection – this latter assumption being expressed by letting the diffusion coefficient $D = 0$ and being an admissible one for an isotropic explosion. So, the mechanical model stated in equation (1) is reduced to:

$$\begin{cases}
\dfrac{\partial \rho}{\partial t} + \dfrac{\partial (\rho v)}{\partial r} = -\dfrac{2\rho v}{r} \\
\dfrac{\partial}{\partial t}(\rho v) + \dfrac{\partial}{\partial r}(\rho v^2 + p) = -\dfrac{2\rho v^2}{r} \\
\dfrac{\partial}{\partial t}(\rho \omega_A) + \dfrac{\partial}{\partial r}(\rho \omega_A v) = -\dfrac{2\rho v \omega_A}{r} - \alpha \omega_A, \\
\qquad\qquad \text{since} \quad r_A = -\alpha \omega_A
\end{cases} \tag{2}$$

It is important to keep in mind that, in the particular problem addressed in this work, a decay in the concentration of the constituent *A* in the mixture (the pollutant) is taken into account in the term r_A. In equation (2) a constitutive relation to describe the rate of pollutant production – accounting for generation or destruction of pollutant, which may be caused by chemical reactions – is assumed as $r_A = -\alpha \omega_A$, where α is a constant. This particular constitutive equation gives rise to a decay in the pollutant concentration along the time.

System (2) may be rewritten by considering $F \equiv \rho$, $G \equiv \rho v$, $H \equiv \rho \omega_A$ as

$$\begin{aligned}
&\frac{\partial F}{\partial t} + \frac{\partial G}{\partial r} = -\frac{2}{r} G \\
&\frac{\partial G}{\partial t} + \frac{\partial}{\partial r}\left(\frac{G^2}{F} + p \right) = -\frac{2}{r}\frac{G^2}{F} \\
&\frac{\partial H}{\partial t} + \frac{\partial}{\partial r}\left(\frac{GH}{F} \right) = -\frac{2}{r}\frac{GH}{F} - \alpha \frac{H}{F}
\end{aligned} \tag{3}$$

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

3. Numerical procedure

In this section a scheme, developed to simulate nonlinear hyperbolic problems, is employed to obtain numerical approximations for the nonlinear system of partial differential equations described in equations (3). Two main

ingredients have been used to achieve this goal: an operator splitting technique together with the Glimm's scheme, successfully employed in the simulation of other nonlinear hyperbolic problems. The procedure consists in a decomposition of the operator in such a way that its merely hyperbolic part is split away from its 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 solution of 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 (see (Freitas Rachid et al, 1994) and references therein). Other relevant examples that could be quoted are the response of non-linear elastic rods (Saldanha da Gama, 1990) and the isothermal and non-isothermal flow of either ideal or Newtonian fluids through unsaturated porous media – covering most one-dimensional cases of interest (see (Martins-Costa et al., 2001) and references therein). It is remarkable that the problems addressed in these works, due to their hyperbolic nature, do not require boundary conditions. They are essentially initial value problems (John, 1982).

Glimm's method, which deals with the homogeneous part of the hyperbolic operator represented in equation (3), employs the solution of the associated Riemann problem to march from a time n to a time $n+1$. Before using Glimm's scheme for solving equations (3) with appropriated initial data, the solution of the associated Riemann problem must be known. 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 arbitrary initial condition given by a function of the position r is approximated by piecewise constant functions, known as 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 for each two consecutive steps [MAR, 03]. The main idea behind the method is to appropriately gather the solution of as many Riemann problems as desired to successively march from time $t = t_n$ to time $t_{n+1} = t_n + \Delta t$.

The first step consists in obtaining an initial approximation for (F, G, H) by advancing Δt in time through the homogeneous (merely hyperbolic) part of the operator via Glimm's method, using the values of (F, G, H) at time $t = t_n$ as initial data. The numerical approximation for the solution at time $t = t_n$ is then obtained by advancing in time with the same time step Δt 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 $t = t_n$ to $t = t_{n+1}$ may be defined as:

$$\left.\begin{aligned} &\frac{\partial F}{\partial t} + \frac{\partial G}{\partial r} = -\frac{2}{r} G \\ &\frac{\partial G}{\partial t} + \frac{\partial}{\partial r}\left(\frac{G^2}{F} + p\right) = -\frac{2}{r}\frac{G^2}{F} \\ &\frac{\partial H}{\partial t} + \frac{\partial}{\partial r}\left(\frac{GH}{F}\right) = -\frac{2}{r}\frac{GH}{F} - \alpha\frac{H}{F} \end{aligned}\right| \quad \left.\begin{aligned} F &= \hat{F}_n(r) \\ G &= \hat{G}_n(r) \\ H &= \hat{H}_n(r) \end{aligned}\right\} \text{at } t = t_n \tag{4}$$

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

3.1. Operator splitting technique

The fist step to approximate the fields F, G and H at the time $t = t_{n+1}$ in the non-homogeneous problem described in equation (4) is to employ an operator splitting technique, described in details by [MAR, 01]. It consists of a decomposition of the operator defined in equation (4) 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 Δt 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) at time t_{n+1} is finally reached by advancing in time to solve the following time evolutionary problem, with the same step $\Delta t = t_{n+1} - t_n$ through equations:

$$\left\{\begin{array}{l}\dfrac{\partial F}{\partial t}=-\dfrac{2}{r}G \\ \dfrac{\partial G}{\partial t}=-\dfrac{2}{r}\dfrac{G^2}{F} \\ \dfrac{\partial H}{\partial t}=-\dfrac{2}{r}\dfrac{GH}{F}-\alpha\dfrac{H}{F}\end{array}\right. \qquad \left.\begin{array}{l}F=\hat{F}_{n+1}(r) \\ G=\hat{G}_{n+1}(r) \\ H=\hat{H}_{n+1}(r)\end{array}\right\} \text{ at } t=t_n \tag{5}$$

as follows:

$$\begin{aligned} F=\hat{F}_{n+1}(r) &\approx \tilde{F}_{n+1}(r)-\left\{\frac{2}{r}\tilde{G}_{n+1}(r)\right\}\Delta t \\ G=\hat{G}_{n+1}(r) &\approx \tilde{G}_{n+1}(r)-\left\{\frac{2}{r}\frac{\left[\tilde{G}_{n+1}(r)\right]^2}{\tilde{F}_{n+1}(r)}\right\}\Delta t \\ H=\hat{H}_{n+1}(r) &\approx \tilde{H}_{n+1}(r)-\left\{\frac{2}{r}\frac{\tilde{G}_{n+1}(r)\tilde{H}_{n+1}(r)}{\tilde{F}_{n+1}(r)}+\alpha\frac{\tilde{H}_{n+1}(r)}{\tilde{F}_{n+1}(r)}\right\}\Delta t \end{aligned} \tag{6}$$

3.2. Glimm's scheme

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

$$\left\{\begin{array}{l}\dfrac{\partial F}{\partial t}+\dfrac{\partial G}{\partial r}=0 \\ \dfrac{\partial G}{\partial t}+\dfrac{\partial}{\partial r}\left(\dfrac{G^2}{F}+p\right)=0 \\ \dfrac{\partial H}{\partial t}+\dfrac{\partial}{\partial r}\left(\dfrac{GH}{F}\right)=0\end{array}\right. \qquad \left.\begin{array}{l}F=\hat{F}_n(r) \\ G=\hat{G}_n(r) \\ H=\hat{H}_n(r)\end{array}\right\} \qquad \text{at } t=t_n \tag{7}$$

In other words, $\tilde{F}_{n+1}(r)$, $\tilde{G}_{n+1}(r)$ and $\tilde{H}_{n+1}(r)$ are the solutions of (7) evaluated at the time $t=t_{n+1}$. The main idea behind Glimm's scheme (Smoller, 1983) is to appropriately gather the solution of as many Riemann problems as desired to successively march from time $t=t_n$ to $t=t_{n+1}$. Glimm's scheme, specifically developed to deal with discontinuous problems, preserves the shock waves magnitude and position, within an uncertainty of Δr (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. In order to employ this scheme a piecewise constant function is used to approximate the initial data, as follows:

$$\left.\begin{array}{l}F=\hat{F}_n(r)\approx F_{n_i}=\hat{F}_n(r_i+\theta_n\Delta r) \\ G=\hat{G}_n(r)\approx G_{n_i}=\hat{G}_n(r_i+\theta_n\Delta r) \\ H=\hat{H}_n(r)\approx H_{n_i}=\hat{H}_n(r_i+\theta_n\Delta r)\end{array}\right\} \qquad \text{for} \quad r_i-\frac{\Delta r}{2}<r<r_i+\frac{\Delta r}{2} \tag{8}$$

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 ($\Delta r=r_{i+1}-r_i$).

The above approximations for the initial data give rise, for each two consecutive steps, to the following Riemann problem – whose detailed solution is presented in (Martins-Costa and Saldanha da Gama, 2003):

$$\left.\begin{aligned}&\frac{\partial F}{\partial t}+\frac{\partial G}{\partial r}=0\\&\frac{\partial G}{\partial t}+\frac{\partial}{\partial r}\left(\frac{G^2}{F}+p(F)\right)=0\\&\frac{\partial H}{\partial t}+\frac{\partial}{\partial r}\left(\frac{GH}{F}\right)=0\end{aligned}\right\}\quad\begin{cases}(F,G,H)=\left(F_{n_i},G_{n_i},H_{n_i}\right)\ \ t=t_n\ ,-\infty<r<r_i+\dfrac{\Delta r}{2}\\(F,G,H)=\left(F_{n_{i+1}},G_{n_{i+1}},H_{n_{i+1}}\right)\ \ t=t_n\ ,\ \mathrm{r}_{i+1}-\dfrac{\Delta r}{2}<r<\infty\end{cases}\tag{9}$$

Denoting by $F_{n_i}^R$ $G_{n_i}^R$, and $H_{n_i}^R$ the generalized solution of the Riemann problem (9), the approximation for the solution of (7) at the time t_{n+1} is given as follows:

$$\begin{aligned}&F=\hat{F}_{n+1}(r)\approx F_{n_i}^R(r,t_{n+1}) &&\mathrm{r}_i<r<r_{i+1}\\&G=\hat{G}_{n+1}(r)\approx G_{n_i}^R(r,t_{n+1}) &&\mathrm{r}_i<r<r_{i+1}\\&H=\hat{H}_{n+1}(r)\approx H_{n_i}^R(r,t_{n+1}) &&\mathrm{r}_i<r<r_{i+1}\end{aligned}\tag{10}$$

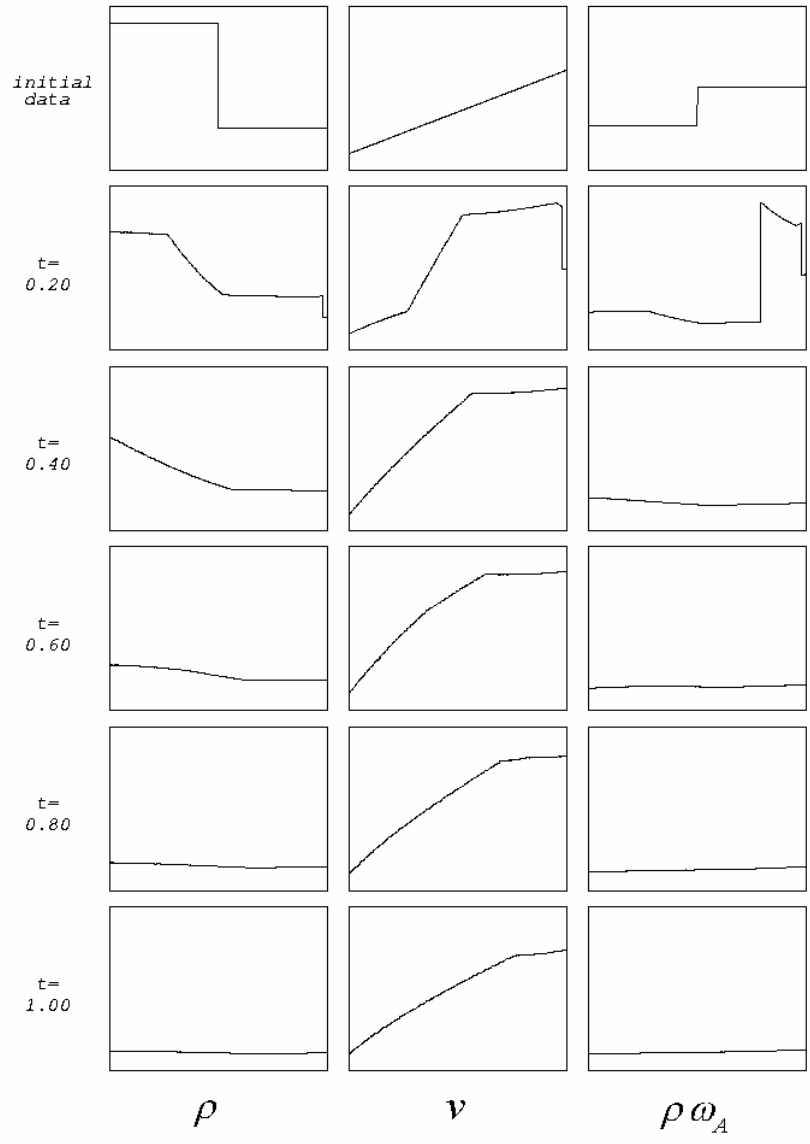

Figure1. Gas density, velocity and pollutant concentration per unit volume variation with position – considering $\alpha=0.01$ and a spherical shell with $r_i=1.00$ and $r_e=2.00$.

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-Friedrich-Lewy (Smoller, 1977) condition is satisfied:

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

where $|\lambda|_{\max}$ is the maximum (in absolute value) propagation speed, considering all the Riemann problems.

At this point a further comment is worth mentioning: the Courant-Friedrich-Lewy condition, expressed in equation (11), although sufficient to assure an adequate treatment of the homogeneous associated problem with absence of interactions among shocks of adjacent Riemann problems, is not sufficient to guarantee the physical validity of the employed operator splitting technique. In the particular problem treated in this work, in which spherical waves are considered, the ratio between the time step Δt and the considered value of the radius *r* must be sufficiently small. In other words, a value ten times smaller than the one computed in equation (11) is employed for the time step Δt, in order to avoid convergence problems.

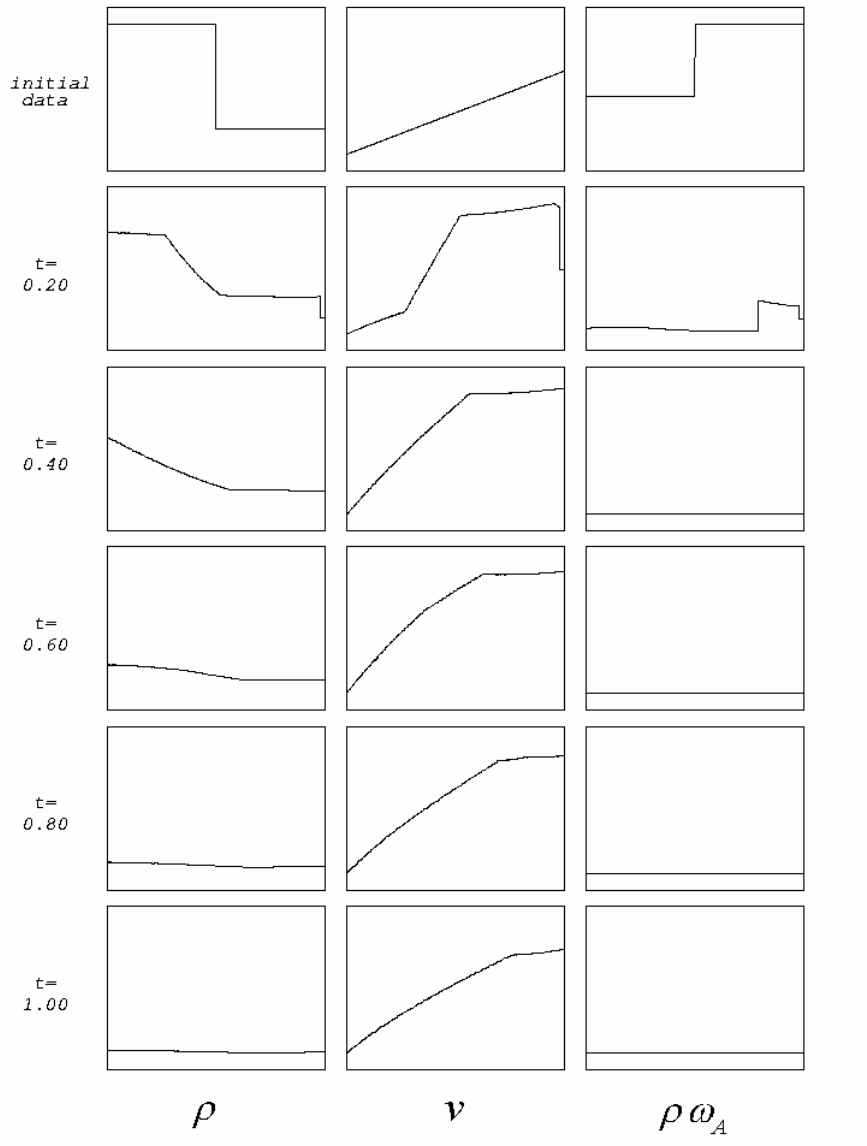

Figure 2. Gas density, velocity and pollutant concentration per unit volume variation with position – considering $\alpha = 10$ and a spherical shell with $r_i = 1.00$ and $r_e = 2.00$.

4. Numerical results and discussion

Figures 1 to 4 show – in all depicted sketches, the evolution of gas density ρ ρ, velocity v and pollutant concentration per unit volume $\rho\omega_A$ along with radial position for five selected time instants. In all the considered cases, the initial data, presented in the three graphs shown in the first line, consists of distinct step functions for gas density ρ (with $\rho_L > \rho_R$) and pollutant concentration in the mixture ω_A (with $\omega_{AL} < \omega_{AR}$), resulting in a pollutant concentration per unit volume given by $\rho\omega_{AL} < \rho\omega_{AR}$.

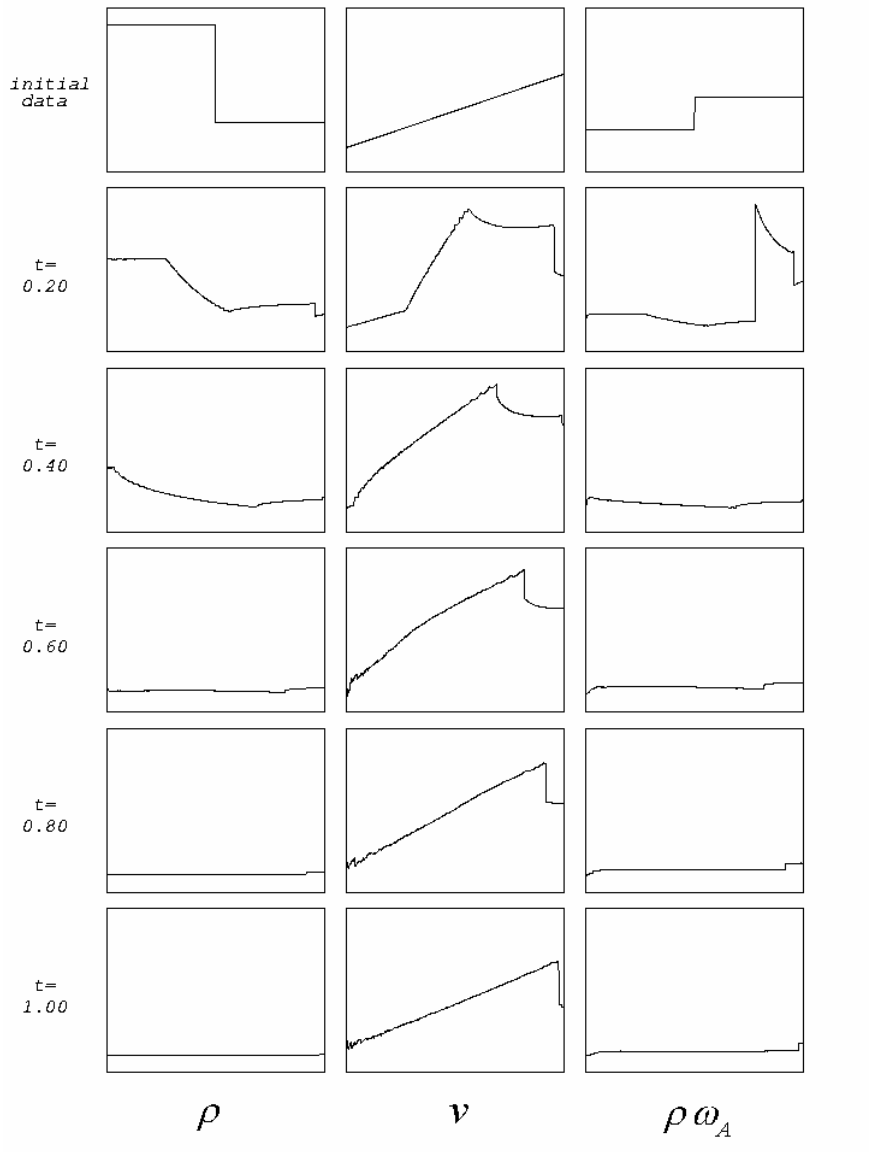

Figure 3. Gas density, velocity and pollutant concentration per unit volume variation with position –considering $\alpha = 0.01$ and a spherical shell with $r_i = 0.01$ and $r_e = 1.01$.

The velocity v initial value is given by a linear increasing function. All these results have been obtained by employing Glimm's difference scheme combined with an operator splitting technique to account for the non-homogeneous portion of the hyperbolic operator and have been achieved with 600 steps.

All results have been obtained by considering a spherical shell unitary thickness. The influence of the behavior of ρ, v $\rho\omega_A$ may be observed by comparing figures 1 (in which the internal and external radii have been made equal to $r_i = 1.00$ and $r_e = 2.00$) and 3 (with $r_i = 0.01$ and $r_e = 1.01$).

In fact, as the spherical shell curvature is increased the effect of the shocks becomes less visible. In other words, a shock dissipation effect could be associated with the curvature increase.

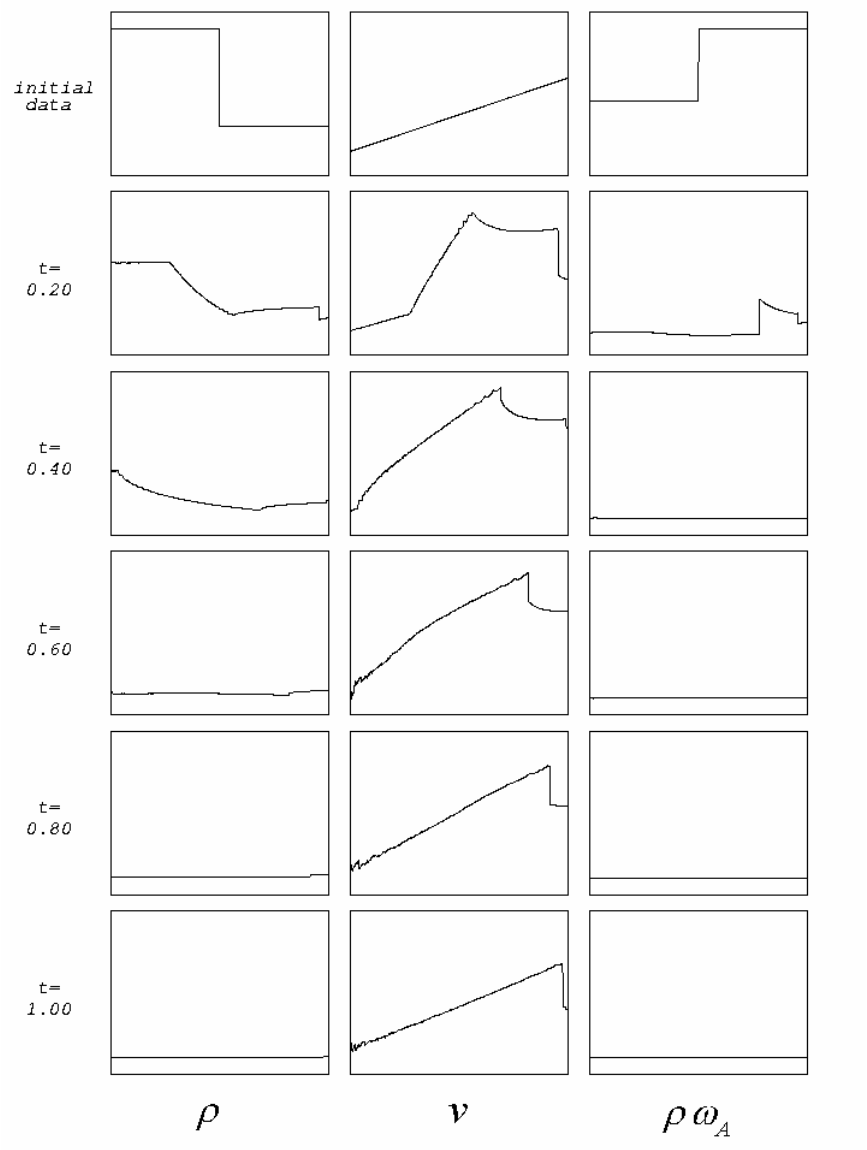

Figure 4. Gas density, velocity and pollutant concentration per unit volume variation with position –considering $\alpha = 10$ and a spherical shell with $r_i = 0.01$ and $r_e = 1.01$.

The influence of the α coefficient may be observed by comparing figure 1 ($\alpha = 0.01$) with figure 2 ($\alpha = 10$) and figures 3 ($\alpha = 0.01$) and 4 ($\alpha = 10$). These results show that the term r_A plays the role of a pollutant sink – giving rise to decay in the pollutant concentration ω_A along the time.

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. Besides, combined with an operator splitting technique this numerical methodology allows the accurate approximation of a nonlinear system of non-homogeneous partial differential equations representing mathematically the transport of a pollutant in the atmosphere in a spherical geometry and accounting for a pollutant generation term (acting in the sense of pollutant destruction) which simulates chemical reactions, causing a damping effect in ω_A variation.

6. Acknowledgement

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