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Glimm Scheme and Operator Splitting for Simulating Radial Transport of a Pollutant in an Atmosphere

Rogério M. Saldanha da Gama[1],Maria Laura Martins-Costa[2]

[1]Mechanical Engineering Department - Universidade do Estado do Rio de Janeiro, Brazil

[2]Laboratory of Theoretical and Applied Mechanics - LMTAMechanical Engineering Department - Universidade Federal Fluminense, Brazil

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ABSTRACT

Aiming to describe transport phenomena in an atmosphere containing a pollutant, assuming radial transport of the pollutant and the atmosphere as an ideal isothermal gas, this work yields a nonlinear hyperbolic system of three partial differential equations that represent mass and momentum conservation for the air-pollutant mixture and the pollutant mass balance. The hyperbolic nature of the system demands a numerical method capable of handling discontinuities. In this context, Glimm's scheme is naturally chosen for the numerical simulation, combined with an operator-splitting technique to account for the non-homogeneous portion of the operator, arising naturally from the problem's spherical geometry.

Nomenclature

F - redefinition of ρ

G - redefinition of ρv

H - redefinition of $\rho\omega_A$

v - air velocity

ρ - air mass density

ρ_A - pollutant mass density

ω_A - pollutant concentration

INTRODUCTION

A preliminary hyperbolic model for radial transport of a pollutant in an isothermal atmosphere is considered in this work. The resulting mathematical representation of this phenomenon is a nonlinear hyperbolic system of three coupled partial differential equations – namely, the mass and momentum conservation laws for the air-pollutant mixture, as well as the pollutant mass balance. After some simplifying assumptions, a set of three coupled nonlinear partial differential equations is obtained, representing the balances of mass and momentum for the air, as well as the pollutant mass balance, with unknowns the air mass density and velocity, and the pollutant concentration fields.

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, to allow 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's hyperbolic feature suggests that it can be approximated using a numerical method specifically designed for discontinuous problems, preserving the shock waves' magnitude and position. Its simulation is

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performed by following a set of systematic procedures 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 the operator splitting into a hyperbolic part and an ordinary one. This operator-splitting technique – necessitated by the problem's intrinsically non-homogeneous nature due to its spherical geometry – is a simple and effective tool that treats 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. This technique has already been successfully employed to approximate other non-linear hyperbolic problems, such as wave propagation in a damageable elasto-viscoplastic pipe and flow through unsaturated porous media. Some representative numerical results are presented to illustrate the responses of both the proposed model and the numerical procedure.

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 to be an ideal gas (all viscosity effects being neglected). The above-mentioned assumptions lead to the following mechanical model to describe the advective-diffusive transport of a pollutant in the air:

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

where 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 constituent *A* in the mixture, ω_A, is defined as the mass fraction of this constituent in the mixture and is expressed by the following equation $\omega_A \equiv \rho_A / \rho$. Besides, D represents the diffusion coefficient of constituent *A* in the mixture and r_A the rate of production of constituent *A*. The most important simplifying assumption is to suppose the presence of a sufficiently small quantity of 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 a convenient redefinition of some variables – ρ is considered 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.

At this point, it is important to state additional simplifying assumptions to be considered in the present work. First, in the absence of chemical reactions that could alter the quantity of the constituent with concentration ω_A, it follows that the production of constituent A $r_A = 0$. Besides, 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 $p'(\rho) > 0$.

In a one-dimensional radial flow, the velocity field may be reduced to a single component in 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 $D = 0$, which is admissible for an isotropic explosion.

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$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{1}{r^2}\dfrac{\partial(\rho r^2 v)}{\partial r} = 0 \\ \rho\dfrac{\partial(\rho v)}{\partial t} + \rho v\dfrac{\partial v}{\partial r} = -p'\dfrac{\partial \rho}{\partial r} + \rho g_r \\ \rho\dfrac{\partial \omega_A}{\partial t} + \rho v\dfrac{\partial \omega_A}{\partial r} = \dfrac{1}{r}\dfrac{\partial}{\partial r}\left(\rho D r^2 \dfrac{\partial \omega_A}{\partial r}\right) + r_A \end{cases} \Rightarrow \begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial(\rho v)}{\partial r} = -\dfrac{2\rho v}{r} \\ \dfrac{\partial}{\partial t}(\rho v) + \dfrac{\partial}{\partial r}(\rho v^2 + p) = -\dfrac{2\rho v^2}{r} \\ \dfrac{\partial}{\partial t}(\rho \omega_A) + \dfrac{\partial}{\partial r}(\rho \omega_A v) = -\dfrac{2\rho v \omega_A}{r} \end{cases} \qquad (2)$$

System (2) may be rewritten by considering:

$F \equiv \rho$, $G \equiv \rho v$, $H \equiv \rho \omega_A$

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

At this point, it is important to note that in order to solve the above problem, initial data for the mass density, velocity, and pollutant concentration are required. Eventually, boundary conditions may also be employed in the solution.

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 with Glimm's scheme, which has been successfully employed to simulate other nonlinear hyperbolic problems. The procedure consists of 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 of 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, as 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 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. 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 this scheme for solving equations (3) with appropriate 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 *x* 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 every two consecutive steps. The main idea behind the method is to appropriately compute the solution of as many Riemann problems as desired, successively marching from time $t = t_n$ to time $t_{n+1} = t_n + \Delta t$.

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The first step consists of 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 $t=t_{n+1}$ is then obtained by advancing in time with the same time step Δt through the purely time-evolutionary system. This procedure is repeated until the specified simulation time is reached.

The numerical procedure employed to advance from the time $t=t_n$ to $t=t_{n+1}$ may be defined as:

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

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

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 Martins-Costa and Saldanha da Gama (2001). 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:

$$\left\{\begin{aligned}
&\frac{\partial F}{\partial t}=-\frac{2}{r}G\\
&\frac{\partial G}{\partial t}=-\frac{2}{r}\frac{G^2}{F}\\
&\frac{\partial H}{\partial t}=-\frac{2}{r}\frac{GH}{F}
\end{aligned}\right.\quad \text{with}\quad \left.\begin{aligned}
&F=\hat{F}_{n+1}(r)\\
&G=\hat{G}_{n+1}(r)\\
&H=\hat{H}_{n+1}(r)
\end{aligned}\right\}\quad \text{at}\quad t=t_n \qquad (5)$$

as follows:

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

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

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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:

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

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 Δx (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 offers a clear advantage in reducing computer storage requirements compared to other methodologies, such as the finite element method 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:

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

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 (2001):

$$\begin{array}{l}\dfrac{\partial F}{\partial t}+\dfrac{\partial G}{\partial r}=0\\ \dfrac{\partial G}{\partial t}+\dfrac{\partial}{\partial r}\left(\dfrac{G^2}{F}+p(F)\right)=0\\ \dfrac{\partial H}{\partial t}+\dfrac{\partial}{\partial r}\left(\dfrac{GH}{F}\right)=0\\ (F,G,H)=(F_{n_i},G_{n_i},H_{n_i}) \qquad \text{for } t=t_n\ , \quad -\infty<r<r_i+\dfrac{\Delta r}{2}\\ (F,G,H)=(F_{n_{i+1}},G_{n_{i+1}},H_{n_{i+1}}) \qquad \text{for } t=t_n\ , \quad r_{i+1}-\dfrac{\Delta r}{2}<r<\infty\end{array} \tag{9}$$

Denoting by $F^R_{n_i}$ $G^R_{n_i}$, and $H^R_{n_i}$ 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:

$$\begin{array}{ll}F=\hat{F}_{n+1}(r)\approx F^R_{n_i}(r,t_{n+1}) & \text{for } r_i<r<r_{i+1}\\ G=\hat{G}_{n+1}(r)\approx G^R_{n_i}(r,t_{n+1}) & \text{for } r_i<r<r_{i+1}\\ H=\hat{H}_{n+1}(r)\approx H^R_{n_i}(r,t_{n+1}) & \text{for } r_i<r<r_{i+1}\end{array} \tag{10}$$

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

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

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

NUMERICAL RESULTS AND DISCUSSION

Figures 1 to 3 show, in all depicted sketches, the evolution of gas density ρ, velocity v, and pollutant concentration per unit volume $\rho\omega_A$ along with radial position at five selected time instants. These results have been obtained by employing Glimm's difference scheme combined with an operator splitting technique to account for the nonhomogeneous portion of the hyperbolic operator – arising naturally in the considered spherical geometry. In all these considered cases, initial data for gas density, velocity, and concentration are presented in the three graphs shown in the first line, and the results were obtained with 300 steps.

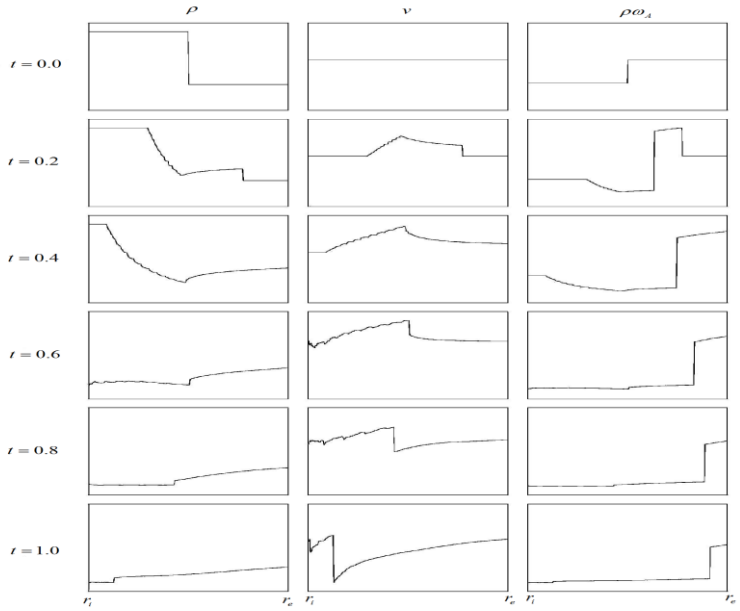

Figure 1. Variation in gas density, velocity, and pollutant concentration per unit volume with radial position. Initial data: step function for ρ, zero v, and step function for ω_A. Spherical shell with $r_i = 0.01$ and $r_e = 1.01$.

In all figures, the initial data consist of a constant value for the velocity $(v = 0)$, while shocks located near the middle of the unitary thickness spherical shell are prescribed for both the mass density (with $\rho_L > \rho_R$) and the concentration of the constituent A in the mixture ω_A (with $\omega_{AL} < \omega_{AR}$), in such a way that the pollutant concentration per unit volume $\rho\omega_A$ is characterized by initial data satisfying $\rho\omega_{AL} < \rho\omega_{AR}$.

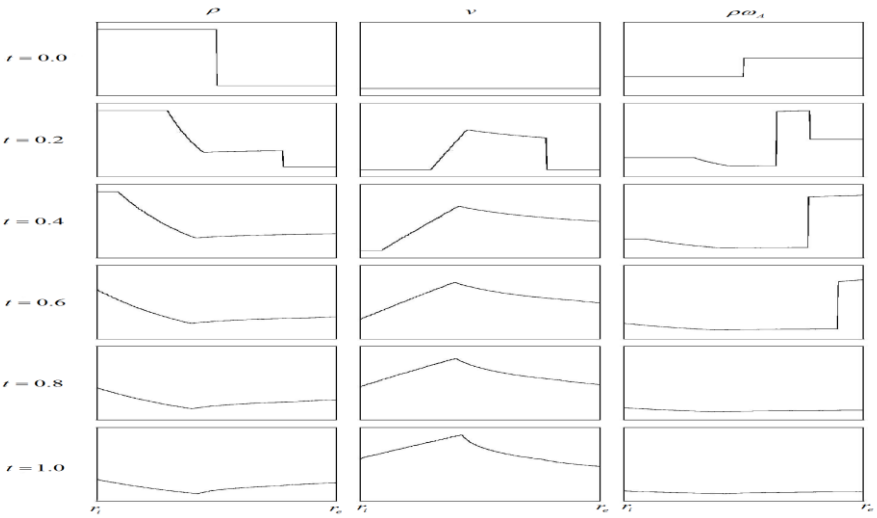

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Figure 2. Variation in gas density, velocity, and pollutant concentration per unit volume with radial position. Initial data: step function for ρ, zero v, and step function for ω_A. Spherical shell with $r_i = 1.00$ and $r_e = 2.00$.

Results have been obtained by considering a spherical shell with unitary thickness. The influence of curvature on the behavior of ρ, v, and $\rho\omega_A$ may be observed by comparing the three figures.

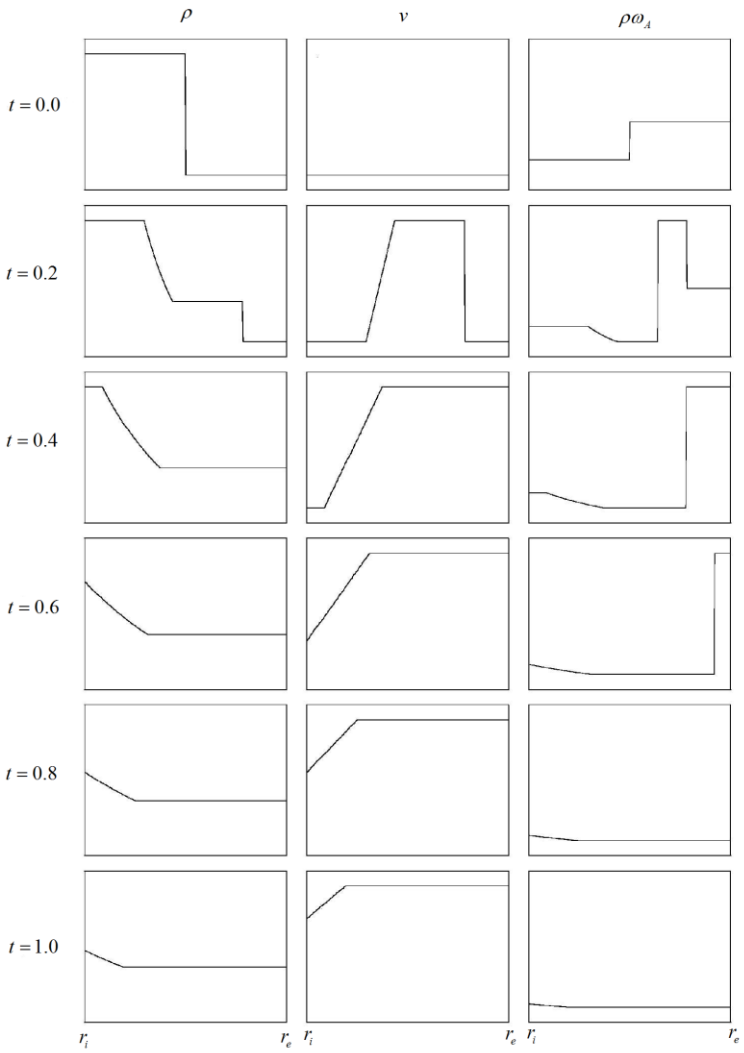

Figure 3. Variation og gas density, velocity, and pollutant concentration per unit volume variation with radial position. Initial data: step function for ρ, zero v, and step function for ω_A. Spherical shell with infinite radius.

Figures 1 to 3 show that as the spherical shell's curvature increases, the shocks become less visible. In fact, the shock-dissipation effect could be associated with an increase in curvature.

CONCLUSIONS

Glimm's method, besides preserving the magnitudes and positions of shock waves, is a convenient tool for solving one-dimensional nonlinear problems, exhibiting features such as low storage requirements and low computational effort compared to other numerical methods for approximating them. Besides, combined with an operator splitting technique, this numerical methodology allows the accurate approximation of a nonlinear system of non-homogeneous partial differential equations that models (mathematically) the transport of a pollutant in the atmosphere in a spherical geometry.

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