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SIMULATION OF RADIAL POLLUTANT MOTION IN POLYTROPIC ATMOSPHERES ACCOUNTIG FOR POLLUTANT DECAY

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Abstract. *A hyperbolic model, that admits discontinuities in addition to smooth or classical solutions, describes the radial motion and decay of a pollutant immersed in a polytropic atmosphere, resulting from mass and momentum conservation for the air-pollutant mixture and the pollutant mass balance. The numerical approximation combines Glimm's method (requiring the solution of a Riemann problem for each two consecutive steps) with an operator splitting technique. Some representative results considering a spherical shell configuration are presented.*

Keywords: *Glimm's scheme, operator splitting, pollutant transport, polytropic atmosphere.*

1. INTRODUCTION

The study of transport phenomena in an environment representing an air-pollutant mixture is justified by the increasingly conscious behavior concerning pollution impact in quotidian and future life. This work employs a preliminary hyperbolic model, in which the atmosphere is treated as an ideal polytropic gas (since meteorological phenomena generally assume adiabatic processes (Jacobson, 2000)), to describe the radial transport of a pollutant in the atmosphere. Assuming the pollutant mass negligible with respect to the air mass, the mathematical representation consists of a nonlinear non-homogeneous system of hyperbolic partial differential equations of mass and momentum balances for the air and the pollutant mass balance that admits discontinuous solutions, in addition to classical smooth ones. The numerical methodology used in this work consists of three distinct ingredients, namely an operator splitting technique, Glimm's scheme and the solution of the associated Riemann problem (see Martins-Costa and Saldanha da Gama, 2006, and references therein).

Riemann problems are may be used to solve systems modeling distinct problems as the evolution of a fluid flow in a nozzle with discontinuous cross-section (Goatin and Le Floch, 2004), the flow of compressible gas in a porous bed, focusing on the solution of a shock-tube problem that also includes a discontinuous jump in the porosity of the bed (Lowe, 2005), hyperelastic solid mechanics (Miller, 2003), or the traffic on a road with points of entry and exit (Mercier, 2009), in which the Riemann problem is solved for the junctions.

Glimm's scheme is implemented by assembling a previously chosen number of Riemann problems to advance in time. Ruan et al. (2008) studied blood flow in a vessel, modeled as an initial-boundary-value problem of a system of hyperbolic, partial-differential equations. Assuming appropriate simplifying hypotheses, they found a global solution using Glimm's finite-difference scheme. Hong and Su (2010) employed a generalized Glimm scheme to find weak solutions of the initial-boundary value problem of hyperbolic systems, construct approximate solutions of Riemann problems, obtaining stable and consistent schemes.

2. PROBLEM STATEMENT AND SIMULATION

In this article the transport of a pollutant in the air is described combining mass and linear momentum conservation for the air-pollutant mixture with mass balance for the pollutant and assuming the mass transfer caused by an advection-diffusion process of the pollutant (A constituent) in the air (supposed as an ideal gas) and the existence of a very small quantity of the pollutant in the mixture at any time instant, with the pollutant mass negligible with respect to the air mass, 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 defining 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. The concentration of the constituent A in the mixture, $\omega_A \equiv \omega$, is defined as the mass fraction of this constituent in the mixture ($\omega \equiv \rho_A / \rho$). Besides, D represents the diffusion coefficient of the constituent A in the mixture and r_A, the rate of production of the constituent A. This latter term, accounting for generation or destruction of pollutant, which may be caused by chemical reactions, will be described by the following constitutive assumption $r_A = -\alpha\omega$, where α is a constant. Some additional simplifying assumptions are: the pressure is function solely of the mass density $p = \hat{p}(\rho)$ with $p'(\rho) > 0$ being its derivative with respect to ρ, the flow is reduced to a radial flow through the spherical shell, so that $\mathbf{v}=v\mathbf{e}_r$; besides both gravitational effects are omitted and diffusion effects are neglected with respect to advection ones. So, Eq. (1a) is reduced to Eq. (1b)

$$\begin{aligned}&\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{v})=0\\&\frac{\partial(\rho\mathbf{v})}{\partial t}+\nabla\cdot(\rho\mathbf{v}\mathbf{v})=-\nabla p+\rho\mathbf{g}\\&\frac{\partial(\rho\omega)}{\partial t}+\nabla\cdot(\rho\omega\mathbf{v})=\nabla\cdot(\rho D\,\nabla\omega)+r_A\end{aligned}\quad\Rightarrow\quad\begin{cases}\dfrac{\partial\rho}{\partial t}+\dfrac{\partial(\rho v)}{\partial r}=-\dfrac{2\rho v}{r}\\\dfrac{\partial}{\partial t}(\rho v)+\dfrac{\partial}{\partial r}(\rho v^2+p)=-\dfrac{2\rho v^2}{r}\\\dfrac{\partial}{\partial t}(\rho\omega_A)+\dfrac{\partial}{\partial r}(\rho\omega v)=-\dfrac{2\rho v\omega_A}{r}-\alpha\omega\end{cases}\tag{1}$$

The numerical simulation employs a methodology developed for problems with discontinuous solutions that consists in treating the non-homogeneous problem sequentially, by combining Glimm's scheme, applied to the homogeneous portion (I) and an operator splitting technique to approximate the time-evolution part (II), as follows

$$(\mathrm{I})\begin{cases}\dfrac{\partial}{\partial t}(\rho)+\dfrac{\partial}{\partial r}(\rho v)=0\\\dfrac{\partial}{\partial t}(\rho v)+\dfrac{\partial}{\partial r}(\rho v^2+p)=0\\\dfrac{\partial}{\partial t}(\rho\omega)+\dfrac{\partial}{\partial r}(\rho\omega v)=0\end{cases}\quad t=t_n\begin{cases}(\rho)=\overline{(\rho)}_n\\(\rho v)=\overline{(\rho v)}_n\\(\rho\omega)=\overline{(\rho\omega)}_n\end{cases}\quad(\mathrm{II})\begin{cases}\dfrac{\partial}{\partial t}(\rho)=-\dfrac{2\rho v}{r}\\\dfrac{\partial}{\partial t}(\rho v)=-\dfrac{2\rho v^2}{r}\\\dfrac{\partial}{\partial t}(\rho\omega)=-\dfrac{2\rho v\omega_A}{r}-\alpha\omega\end{cases}\quad t=t_n\begin{cases}(\rho)=\overline{\overline{(\rho)}}_{n+1}\\(\rho v)=\overline{\overline{(\rho v)}}_{n+1}\\(\rho\omega)=\overline{\overline{(\rho\omega)}}_{n+1}\end{cases}\tag{2}$$

In brief, initial approximations for the fields ρ, ρv and $\rho\omega$ are obtained with Glimm's scheme, implemented by assembling a previously chosen number of Riemann problems to advance from time n to time n+1 (Smoller, 1983; John, 1982). In the sequence, the "prediction" is "corrected": the results at time n+1 are obtained by solving the above system (II), using the results obtained in (I) as initial estimates, with the same time step. The methodology, described in details in Martins-Costa and Saldanha da Gama (2006), has been previously applied to a homogeneous system (Martins-Costa and Saldanha da Gama, 2003) and to non-homogeneous systems of two non-linear equations describing flow though unsaturated porous media (Martins-Costa and Saldanha da Gama, 2003).

3. RESULTS

Four different problems are presented, in which the effects of the pollutant decay coefficient α and the spherical shell curvature are considered. In all these problems, with the same initial data are assumed, being given by a constant mass density ρ, a step function for the velocity (with $v_L<v_R$) and a step function for the pollutant concentration per unit volume (with $\rho\omega_L>\rho\omega_R$).

Figures 1 to 4 contain four distinct figures; six lines and three columns of graphs compose the top left set, each line representing a distinct time instant (the first one being the initial condition), and each a distinct variable; the vertical axis corresponds to the numerical value assumed by the variables (ρ, v and $\rho\omega$), the horizontal one being the spatial coordinate, with the internal radius placed at the left-hand side and the external radius at the right one. The behavior of ρ, ρv and $\rho\omega$ is also depicted in the 3-D diagrams, represented on the top right (ρ), bottom left (v) and bottom right ($\rho\omega$). In all 3-D diagrams the smallest values are depicted in dark blue while the highest are in dark brown.

The effects of the decay coefficient α may be noted by comparing figures 1 (α=0.01) and 2 (α=10), for r_i= 1 and r_e=2; and figures 3 (α=0.01) and 4 (α=10) , for r_i= 0.01 and r_e=1.01, which show a decay of the pollutant concentration along the time as α increases (r_A acting as a pollutant source). Comparing figures 1 and 3 and 2 and 4 the effect of the spherical shell curvature may be noted, since in all cases a unitary thickness is considered. As the curvature increases, the effect of the shocks decreases, in other words, a dissipative effect may be associated to the curvature increase.

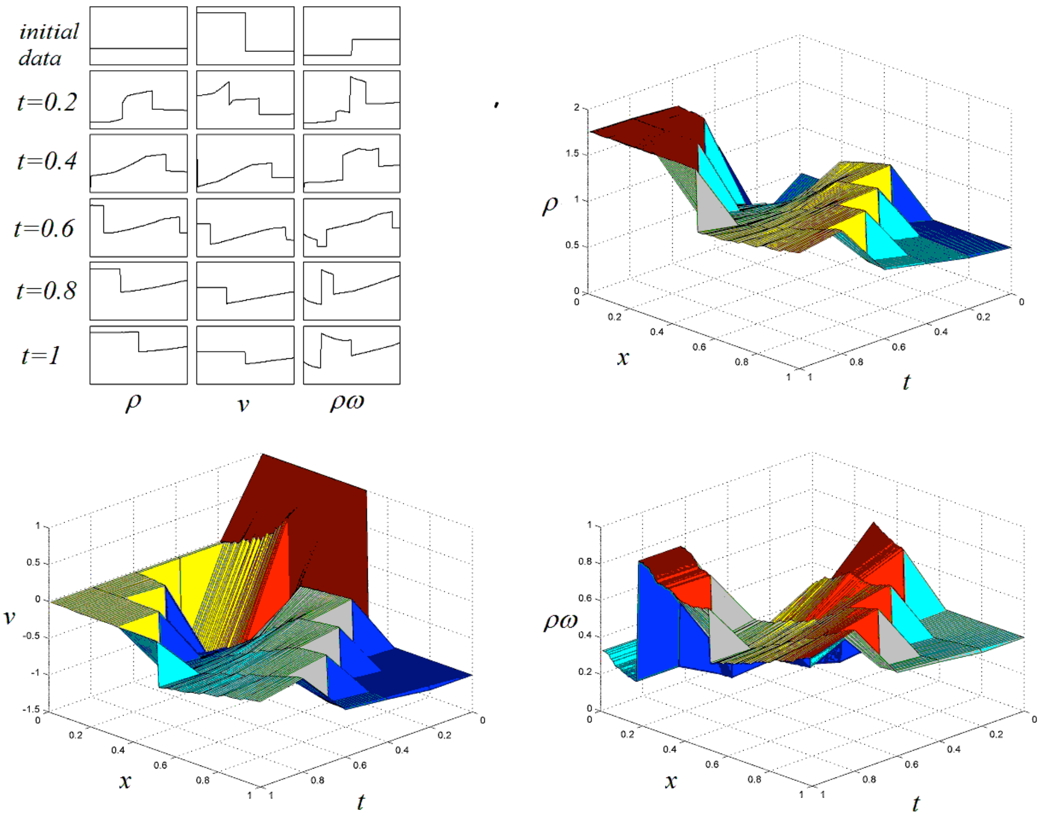

Figure 1. Gas density, velocity and pollutant concentration per unit volume variation with position – considering $\alpha = 0.01$ and a spherical shell with $r_i = 1$ and $r_e = 2$.

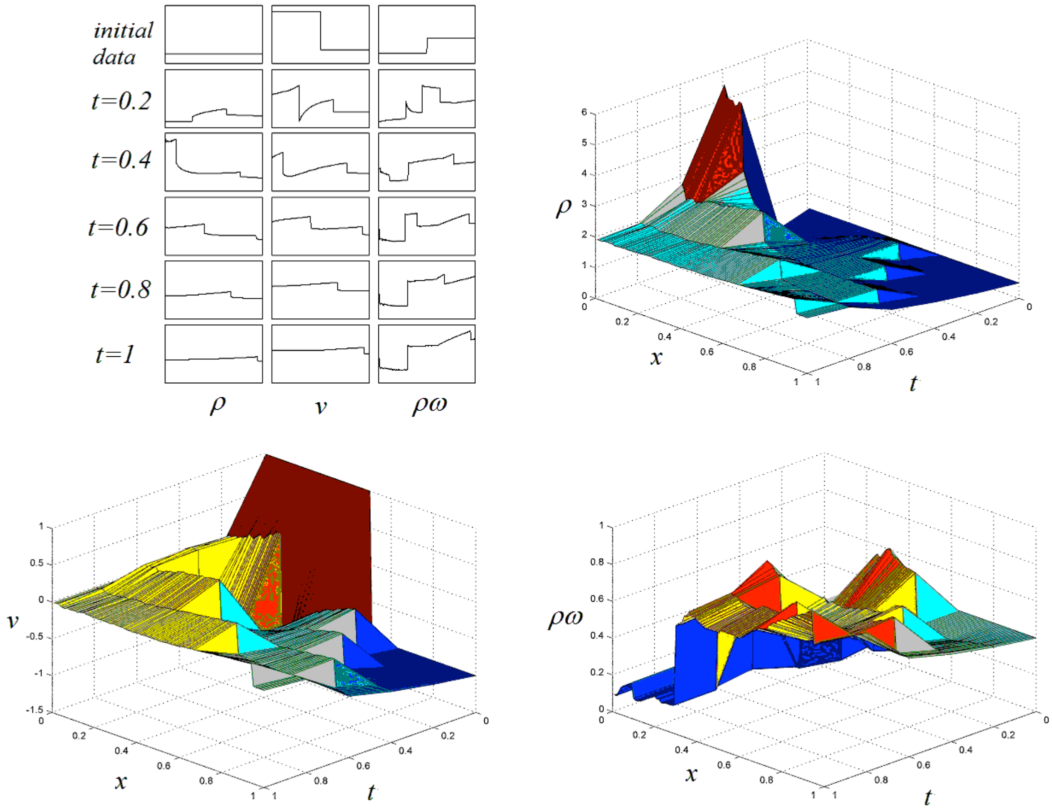

Figure 2. Gas density, velocity and pollutant concentration per unit volume variation with position – considering $\alpha = 10$ and a spherical shell with $r_i = 1$ and $r_e = 2$.

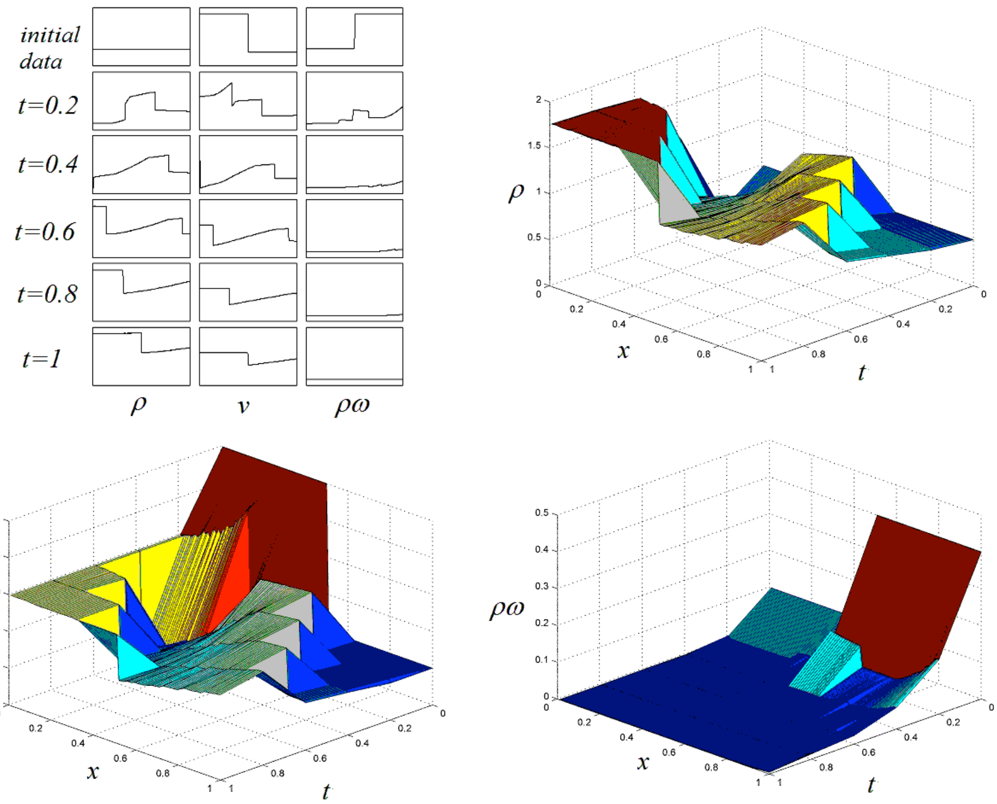

Figure 3. Gas density, velocity and pollutant concentration per unit volume variation with position – considering $\alpha = 0.01$ and a spherical shell with $r_i = 0.01$ and $r_e = 1.001$.

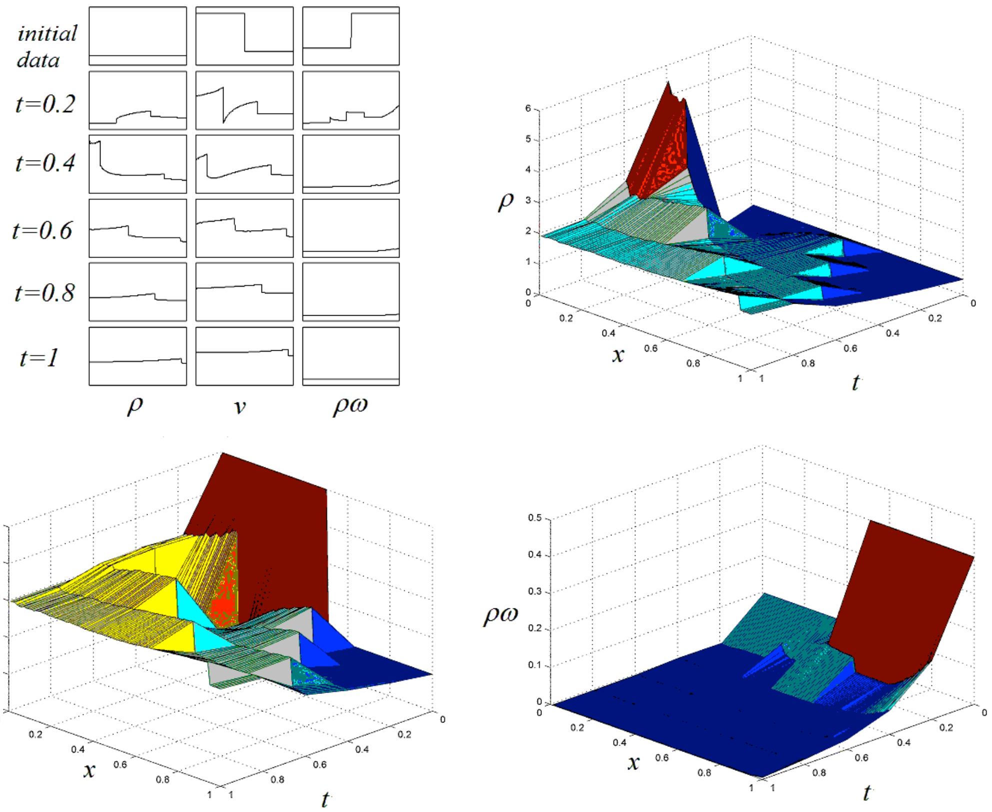

Figure 4. Gas density, velocity and pollutant concentration per unit volume variation with position – considering $\alpha = 10$ and a spherical shell with $r_i = 0.01$ and $r_e = 1.001$.

4. FINAL REMARKS

The numerical methodology presented in this work – combining Glimm's scheme and an operator splitting technique to deal with the non-homogeneous portion of the hyperbolic operator – allowed the accurate approximation of a nonlinear and non-homogeneous system of three partial differential equations representing mathematically the transport of a pollutant in the atmosphere and accounting for the pollutant decay.

Glimm's method presents no numerical dissipation, preserving shock waves magnitude and position. Besides, when compared with other numerical procedures to approximate nonlinear problems, it has lower storage costs and requires lower computational effort.

5. ACKNOWLEDGEMENTS

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