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ONEDIMENSIONAL SIMULATION OF POLLUTANT TRANSPORT IN AN ISOTHERMAL ATMOSPHERE WITH SHOCK WAVES

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Abstract. *A model for the transport of a pollutant in the atmosphere is presented by considering mass and linear momentum conservation for the air-pollutant mixture as well as the mass balance for the pollutant. The resulting mathematical description consists of a nonlinear system of hyperbolic equations which admits discontinuities in addition to smooth or classical solutions. In the particular case of an initial value problem characterized by step functions for both the velocity and the pollutant concentration fields and constant mass density as initial data, the associated Riemann problem may be analytically solved.*

Keywords: *Pollutant transport, isothermal atmosphere, Riemann problem, shock waves.*

1. INTRODUCTION

Most transport phenomena are modeled under assumptions, which give rise to parabolic or elliptic partial differential equations – which always admit regular solutions whose simulation may employ well known numerical tools. Examples of usual procedures to simulate such phenomena are finite elements, finite differences or finite volumes.

In this work a distinct approach is carried out. A mathematical modeling for a given transport phenomenon (the transport of a pollutant in the air) is presented, giving rise to a set of nonlinear partial differential hyperbolic equations. Such a description admits – besides the usual continuous solutions – discontinuous ones, which, in general, present shock waves. This system is obtained by considering, besides mass and linear momentum conservation for the air-pollutant mixture – the classical equations of gas dynamics – the mass balance for the pollutant.

The above mentioned approach is quite interesting since, in any real natural phenomenon, the propagation of any quantity – or information – has a finite speed. Unfortunately, the numerical simulation of nonlinear hyperbolic problems is not well performed by employing the classical

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numerical procedures mentioned before, it requires special tools such as, for instance, Glimm's scheme or Godunov's one.

The Riemann problem – associated with a class of problems describing the transport of a pollutant in an ideal gas with constant temperature – consists of a hyperbolic initial value problem subjected to a step function as initial data, which admits analytical generalized solution. It is a fundamental step for employing Glimm's scheme when simulating problems with any initial data and/or boundary condition. Although this Riemann problem may be considered as a step in Glimm's scheme, it has its own physical meaning and, in many cases, it gives sufficient insight for avoiding a numerical simulation.

The main goal of this article is to present an analytical solution for the associated Riemann problem in the particular case when the initial value problem is characterized by initial data in which there are a jumps in both the velocity and the pollutant concentration fields while the mass density remains constant. As it will be shown in the subsequent sections, in this case all the connections between intermediate states are shocks, one of them being a contact shock – a discontinuity with propagation speed corresponding exactly to the associated eigenvalue.

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). Besides, the diffusion process is supposed to be described according to the classical Fick's law. The above stated assumptions lead to the following mechanical model to describe the advective-diffusive transport of a pollutant in the air:

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

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 the constituent *A* in the mixture, w_A, is defined as the mass fraction of this constituent in the mixture, being expressed by the following equation $w_A \equiv r_A / r$. Besides, D represents the diffusion coefficient of the constituent *A* in the mixture, and r_A the rate of production of the constituent *A*. The most important simplifying assumption is to suppose the presence of a sufficiently small quantity of the constituent *A* in the air – 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 of considering mass and momentum equations for the air 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. The balance equations may be rewritten in a more convenient way:

$$
\begin{aligned}
&\frac{\partial r}{\partial t}+\nabla\cdot(r\,\mathbf{v})=0\\
&\frac{\partial(r\,\mathbf{v})}{\partial t}+\nabla\cdot(r\,\mathbf{vv})=-\nabla p+r\,\mathbf{g}\\
&\frac{\partial(rw_A)}{\partial t}+\nabla\cdot(rw_A\mathbf{v})=\nabla\cdot(r\,D\;\nabla w_A)+r_A=0
\end{aligned}
\tag{2}
$$

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 which could alter the quantity of the constituent with concentration w_A, it comes that the production of constituent A, $r_A=0$. Besides, the pressure is considered as being a function of the mass density r only, its derivative with respect to r being given by p'.

Considering a plane flow, the velocity field may be reduced to a single component on the flow direction $\mathbf{v}=v\mathbf{i}$. Besides, assuming a horizontal flow – which allows to omit gravitational effects and also that diffusion effect can be neglected, when compared to advection effect - this latter assumption being expressed by letting the diffusion coefficient $D=0$ – the homogeneous problem associated with equation (2) comes as a natural consequence:

$$
\begin{aligned}
&\frac{\partial r}{\partial t}+\frac{\partial}{\partial x}(r\,v)=0 &&\frac{\partial r}{\partial t}+\frac{\partial(r\,v)}{\partial x}=0\\
&\frac{\partial}{\partial t}(r\,v)+\frac{\partial}{\partial x}(r\,v^2+p)=0 &&\frac{\partial(r\,v)}{\partial t}+\frac{\partial(r\,v^2)}{\partial x}+p'\frac{\partial r}{\partial x}=0\\
&\frac{\partial}{\partial t}(rw_A)+\frac{\partial}{\partial x}(rw_Av)=0 &&\frac{\partial(rw_A)}{\partial t}+\frac{\partial(rw_Av)}{\partial x}=0
\end{aligned}
\tag{3}
$$

A convenient redefinition of variables, $F\equiv r$, $G\equiv r\,v$, $H\equiv rw_A$, allows to express problem (3) as:

$$
\begin{aligned}
&\frac{\partial F}{\partial t}+\frac{\partial G}{\partial x}=0\\
&\frac{\partial G}{\partial t}+\frac{\partial}{\partial x}\left(\frac{G^2}{F}\right)+p'\frac{\partial F}{\partial x}=\frac{\partial G}{\partial t}+\frac{\partial}{\partial x}\left(\frac{G^2}{F}+p\left(F\right)\right)=0\\
&\frac{\partial H}{\partial t}+\frac{\partial}{\partial x}\left(\frac{GH}{F}\right)=0
\end{aligned}
\tag{4}
$$

Problem (4) could also be written in matrix form as:

$$
\frac{\partial}{\partial t}\begin{bmatrix}F\\G\\H\end{bmatrix}+\begin{bmatrix}0 & 1 & 0\\ -\dfrac{G^2}{F^2}+p' & 2\dfrac{G}{F} & 0\\ -\dfrac{GH}{F^2} & \dfrac{H}{F} & \dfrac{G}{F}\end{bmatrix}\frac{\partial}{\partial x}\begin{bmatrix}F\\G\\H\end{bmatrix}=\begin{bmatrix}0\\0\\0\end{bmatrix}
\tag{5}
$$

3. SHOCK WAVES

The study of shock waves phenomenon in a compressible gas requires some simplifying assumptions (Hughes and Marsden, 1976). First the flow is assumed one-dimensional, namely there is a single non-zero velocity component $v = v(x,t)$, the pressure and the mass density being such that $p = p(x,t)$ $r = r(x,t)$. The second important hypothesis is the absence of viscous effects, resulting in the assumption of a perfect fluid – a fluid that can exert no tangential stresses on the surface – the internal product of the stress tensor and the unit outward normal being always parallel to the normal. Finally, the pressure is supposed to be a function of the density only, i.e., $p = p(r)$, p being sufficiently smooth and its derivative being a positive function, i.e., $p' = dp/dr > 0$, thus assuring real wave speeds.

In the presence of a discontinuity, the system in its differential form becomes meaningless, but the balance equations – conservation of mass, momentum and energy – cannot be violated. Their integral form imposes restrictions on the behavior of a shock wave. In order to incorporate all the conditions to be satisfied, weak solutions must be searched, satisfying some conditions. First, the solution of the system is composed by regions – separated by discontinuities that, under certain conditions, may be shocks. Within each region the mass density and the velocity must be smooth functions and the solution of the differential equations are to hold in the classical sense. Another important condition to be satisfied is that the conservation equations in its integral form remain valid at a shock. Finally, the problem must remain physically meaningful when viscosity and thermodynamic effects are accounted for – namely the solution of the simplified problem is supposed to act as a limit case regarding the complete problem. Considering $[\![\mathbf{f}]\!]$, the jump of the variable $\mathbf{f}$ (a vector-valued function) across a smooth curve Σ, the jump condition could be considered as $\left(\mathbf{f}^{+} - \mathbf{f}^{-}\right) \cdot \mathbf{n} = 0$.

The original problem – the transport of a pollutant in the air, supposing the presence of a sufficiently small quantity of the constituent A in the air at any time instant together with the additional hypotheses stated before equation (3) – strong formulation is defined as

$$\begin{aligned}
&\frac{\partial}{\partial t}(r) + \frac{\partial}{\partial x}(rv) = 0 \\
&\frac{\partial}{\partial t}(rv) + \frac{\partial}{\partial x}(rv^2 + p) = 0 \\
&\frac{\partial}{\partial t}(rw_A) + \frac{\partial}{\partial x}(rw_A v) = 0
\end{aligned} \tag{6}$$

A weak formulation could be obtained by considering a given region $\Omega \in \mathbb{R}^2$ and a test function $y\left(x,t\right)$ – a C^{∞} function with compact support. In this case, a corresponding weak formulation could be expressed as:

$$\begin{aligned}
&\int_{\Omega}\left[\frac{\partial y}{\partial t}(r) + \frac{\partial y}{\partial x}(rv)\right] dxdt = 0 \\
&\int_{\Omega}\left[\frac{\partial y}{\partial t}(rv) + \frac{\partial y}{\partial x}(rv^2 + p)\right] dxdt = 0 \\
&\int_{\Omega}\left[\frac{\partial y}{\partial t}(rw_A) + \frac{\partial y}{\partial x}(rw_A v)\right] dxdt = 0
\end{aligned} \tag{7}$$

The corresponding jump condition could be obtained by making $[\![\mathbf{f}]\!]\cdot\mathbf{n}=0$, $\mathbf{n}$ being the outward normal to a smooth curve Σ, as:

$$\begin{cases} s[\![r]\!]=[\![rv]\!] \\ s[\![rv]\!]=[\![rv^2+p]\!] \\ s[\![rw_A]\!]=[\![rw_A v]\!] \end{cases} \Rightarrow \quad s=\frac{[\![rv]\!]}{[\![r]\!]}=\frac{[\![rv^2+p]\!]}{[\![rv]\!]}=\frac{[\![rvw_A]\!]}{[\![rw_A]\!]} \tag{8}$$

in which s represents the shock speed. Equations (8) represent the conservation of mass and momentum for the air-pollutant mixture and the mass balance for the pollutant (the conservation of species w_A) across the shock.

At this point it is important to stress that adding a viscous term to the momentum equation, namely $n\dfrac{\partial^2 v}{\partial x^2}$ in the strong formulation, in which n represents the kinematics viscosity, results in the weak formulation being replaced by

$$\begin{aligned} &\int_\Omega \left[\frac{\partial y}{\partial t}(r)+\frac{\partial y}{\partial x}(rv)\right]dxdt=0 \\ &\int_\Omega \left[\frac{\partial y}{\partial t}(rv)+\frac{\partial y}{\partial x}(rv^2+p)+\frac{\partial^2 y}{\partial x^2}(nv)\right]dxdt=0 \\ &\int_\Omega \left[\frac{\partial y}{\partial t}(rw_A)+\frac{\partial y}{\partial x}(rw_A v)\right]dxdt=0 \end{aligned} \tag{9}$$

The solution of equations (9) does not possess shocks, the effect of viscosity being to smooth out shock waves. It is important to mention that as $n\to 0$ the weak solution of both systems are coincident.

The entropy or shock admissibility condition for equations (7), considering the eigenvalues l_1 and l_3, may be stated as

$$\begin{cases} v^R+\sqrt{p'}^R < s < v^L+\sqrt{p'}^L \\ v^L-\sqrt{p'}^L < s \end{cases} \tag{10}$$

or, alternatively:

$$\begin{cases} v^R-\sqrt{p'}^R < s < v^L-\sqrt{p'}^L \\ \qquad\qquad\quad s < v^R+\sqrt{p'}^R \end{cases} \tag{11}$$

If either (10) or (11) is satisfied the shock is deemed admissible.

4. RIEMANN PROBLEM

The homogeneous problem associated with equation (1), expressed either by equation (3) or (4) or (5), is called a Riemann problem (John, 1982) provided that some conditions are verified. First, the system must be a genuinely non-linear hyperbolic one. In order to ensure this hypothesis, the first derivative of the pressure with respect to the density, p', must be positive. Besides, Riemann problem is a special initial value problem defined by equation (5), which must hold for $-\infty < x < +\infty$, $t > 0$, satisfying the following initial condition:

$$\begin{aligned} (F,G,H) &= (F_L, G_L, H_L) \quad \text{for } x<0 \quad \text{and} \quad t=0 \\ (F,G,H) &= (F_R, G_R, H_R) \quad \text{for } x>0 \quad \text{and} \quad t=0 \end{aligned} \tag{12}$$

So, the variables F, G and H, are functions of both *x* and *t*, being subject to a step function as initial condition – specified in equation (12), where (F_L, G_L, H_L) represent its value at the left-hand side and (F_R, G_R, H_R) its value at the right-hand side. The generalized solution for the above described Riemann problem may be expressed as a function of a similarity variable $x = x/t$, provided that the initial condition is a step function and that the problem is homogeneous. Substituting $x = x/t$, the associated Riemann problem may be expressed as:

$$-x\frac{d}{dx}\begin{bmatrix} F \\ G \\ H \end{bmatrix} + \begin{bmatrix} 0 & 1 & 0 \\ -\dfrac{G^2}{F^2}+p' & 2\dfrac{G}{F} & 0 \\ -\dfrac{GH}{F^2} & \dfrac{H}{F} & \dfrac{G}{F} \end{bmatrix}\frac{d}{dx}\begin{bmatrix} F \\ G \\ H \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad \text{for } -\infty < x < +\infty \tag{13}$$

$$\begin{aligned} (F,G,H) &= (F_L, G_L, H_L) \quad \text{for } x \to -\infty \\ (F,G,H) &= (F_R, G_R, H_R) \quad \text{for } x \to +\infty \end{aligned} \tag{14}$$

the corresponding eigenvalues being given by:

$$l_i = \frac{G}{F} + a_i\sqrt{p'} = v + a_i\sqrt{p'}, \qquad \text{with} \quad a_i = i-2 \tag{15}$$

If it can be assured that $p' > 0$, for all values assumed by the similarity variable x and all time instants t, then equations (13) represent a genuinely nonlinear hyperbolic system and equations (13)-(14) are called a Riemann problem (Martins-Costa and Saldanha da Gama, 2001). The generalized solution of this Riemann problem depends only on the ratio $x = x/t$ being reached by connecting the left state (F_L, G_L, H_L) and the right state (F_R, G_R, H_R) by means of two intermediate states, namely (F_{*1}, G_{*1}, H_{*1}) and (F_{*2}, G_{*2}, H_{*2}) as follows: $(F_L, G_L, H_L) \to (F_{*1}, G_{*1}, H_{*1}) \to (F_{*2}, G_{*2}, H_{*2}) \to (F_R, G_R, H_R)$, in which $*1$ and $*2$ indicate intermediate constant states to be determined. The connection between the states $L \to *1$, $*1 \to *2$ and $*2 \to R$ may be performed either by rarefactions or shocks. 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.

A particular type of link is verified in this problem – the connection between intermediate states $*1$ and $*2$ is a contact shock (Smoller, 1983). This contact shock is characterized by absence of jump for both variables F and G – in such a way that $F_{*1} = F_{*2}$ and $G_{*1} = G_{*2}$. The jump is verified solely for *H*, with a propagation speed $v = H/r$ – the speed assuming the same value of the corresponding eigenvalue. The contact shock may be viewed as a limit-case of rarefaction in which 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. It can be shown that there are no restrictions on the jump of w_A allowing the choice of $[\![w_A]\!]=0$, the connection between the states $*1 \rightarrow *2$ being characterized by $w_{A*1}=w_{AL}$ and $w_{A*2}=w_{AR}$. The presence of this contact shock allows concluding that the pollutant is propagated with a speed v, being carried by the atmosphere. Besides, an important simplification may be considered, which allows the problem reduction to a two variables (v and r) problem with only two connections to be determined, namely, $L \underset{R1 \text{ or } S1}{\Longrightarrow} * \underset{R3 \text{ or } S3}{\Longrightarrow} R$. So, the referred states may be connected either by an *i*-Rarefaction or an *i*-Shock.

5. PROBLEM SOLUTION

In order to illustrate the theory presented in the last section, a semi-infinite region, representing a very large cylinder containing a mixture of a given pollutant with concentration w_A and air – characterizing a hemispace $x<0$ – bounded by an impermeable wall at $x=0$ is considered for a particular situation in which the initial data is characterized by a constant value of mass density r in the whole domain while there is a jump in both the velocity and the concentration fields, with $v_L > v_R$ and $w_{AL} > w_{AR}$ (and, consequently, $rw_{AL} > rw_{AR}$).

This problem illustrates the solution of two consecutive Riemann problems describing the evolution of the fields r (mass density), v (velocity) and rw_A (pollutant concentration per unit mass). The former treating the evolution from the initial time instant $t=0$ until the shock wave on the right-hand side reaches the impermeable wall – thus generating a second Riemann problem – this latter problem beginning when the shock wave reaches the impermeable wall.

Since the gas is compressible, its mass density r is greatly increased in a region near the wall (in the vicinity of the point $x=0$) due to the shock of the field v reaching the wall thus provoking a variation on rw_A. The pollutant distribution depends strongly on the velocity variation being, consequently, affected by the presence of the impermeable wall (stagnation point).

The particular initial data considered in this case gives rise to a generalized solution composed by a 1- Shock, a 3-Shock and a 2-Contact-Shock with speed $s_2 = l_2 = v_*$, associated with the jump in the concentration w_A only. For $x/t < s_2$ it comes that $w_A = w_{AL}$ while for $x/t > s_2$, $w_A = w_{AR}$. This initial value problem is characterized by the existence of an analytical solution for the associated Riemann problem in which all the connections between the states are shocks:

$$L \underset{\text{Shock 1}}{\Longrightarrow} *1 \underset{\text{Contact Shock}}{\Longrightarrow} *2 \underset{\text{Shock 3}}{\Longrightarrow} R$$

In this case, a solution with the connections of the kind 1-Shock – 3-Shock, requires that

$$v_R - v_L = -\sqrt{\left(\frac{1}{r_*}-\frac{1}{r_L}\right)(p_L - p_*)} - \sqrt{\left(\frac{1}{r_*}-\frac{1}{r_R}\right)(p_R - p_*)} \qquad (16)$$

in which the negative signs come from the entropy condition.

Considering an isothermal process, $p = c^2 r$,

$$v_R - v_L = -\sqrt{\left(\frac{1}{r_*}-\frac{1}{r_L}\right)(r_L - r_*)c^2} - \sqrt{\left(\frac{1}{r_*}-\frac{1}{r_R}\right)(r_R - r_*)c^2} \qquad (17)$$

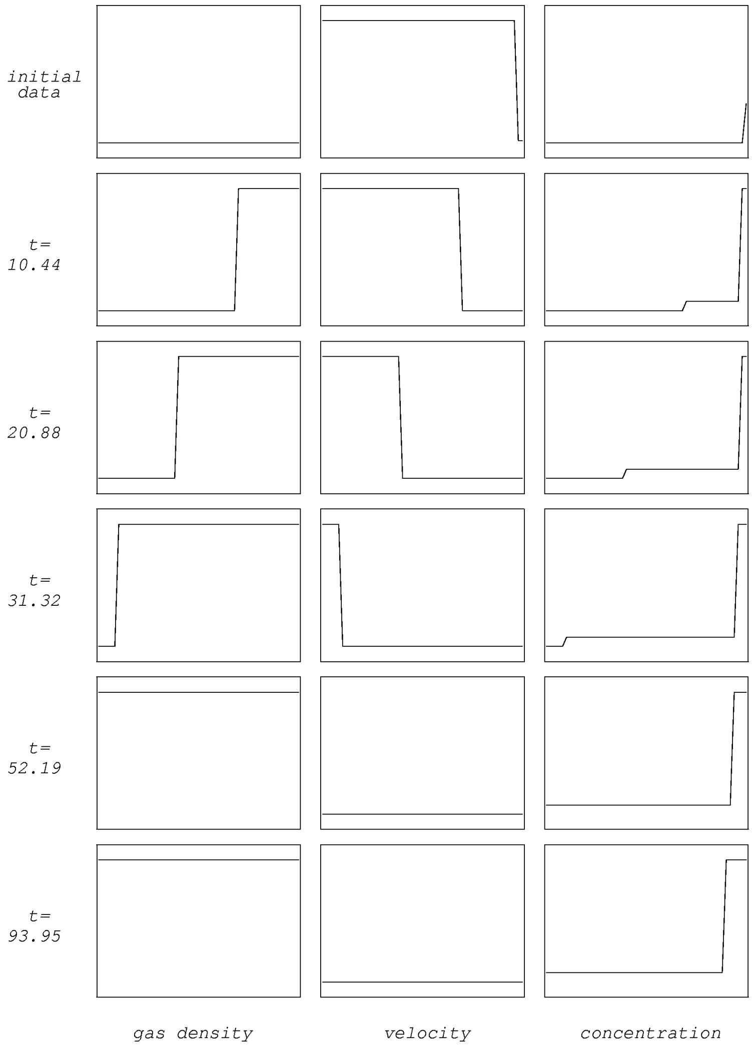

Figure 1. Example of evolution of two consecutive Riemann problems
(initial data: $v_L = 2.5$, $v_R = 0$, $w_{AL} = 0.1$, $w_{AR} = 0.8$ and constant r)

$$v_L - v_R = \sqrt{\frac{(r_L - r_*)}{r_* r_L}(r_L - r_*)c^2} + \sqrt{\frac{(r_R - r_*)}{r_* r_R}(r_R - r_*)c^2} \tag{18}$$

$$v_L - v_R = (r_L - r_*)c\frac{1}{\sqrt{r_*}}\frac{1}{\sqrt{r_L}} + (r_R - r_*)c\frac{1}{\sqrt{r_*}}\frac{1}{\sqrt{r_R}} \tag{19}$$

$$\sqrt{r_*}(v_L - v_R) = (r_L - r_*)\frac{c}{\sqrt{r_L}} + (r_R - r_*)\frac{c}{\sqrt{r_R}} \tag{20}$$

$$\sqrt{r_*}(v_L - v_R) = -r_*\left(\frac{c}{\sqrt{r_L}} + \frac{c}{\sqrt{r_R}}\right) + c\left(\sqrt{r_R} + \sqrt{r_L}\right) \tag{21}$$

$$r_*\left(\frac{c}{\sqrt{r_L}}+\frac{c}{\sqrt{r_R}}\right)-\sqrt{r_*}\,(v_L-v_R)-c\left(\sqrt{r_R}+\sqrt{r_L}\right)=0 \tag{22}$$

which is solved for r_*, giving:

$$r_*=\left\{\frac{(v_R-v_L)+\sqrt{(v_R-v_L)^2+4c^2\left(\frac{1}{\sqrt{r_L}}+\frac{1}{\sqrt{r_R}}\right)\left(\sqrt{r_R}+\sqrt{r_L}\right)}}{\left(\frac{1}{\sqrt{r_L}}+\frac{1}{\sqrt{r_R}}\right)2c}\right\}^2 \tag{23}$$

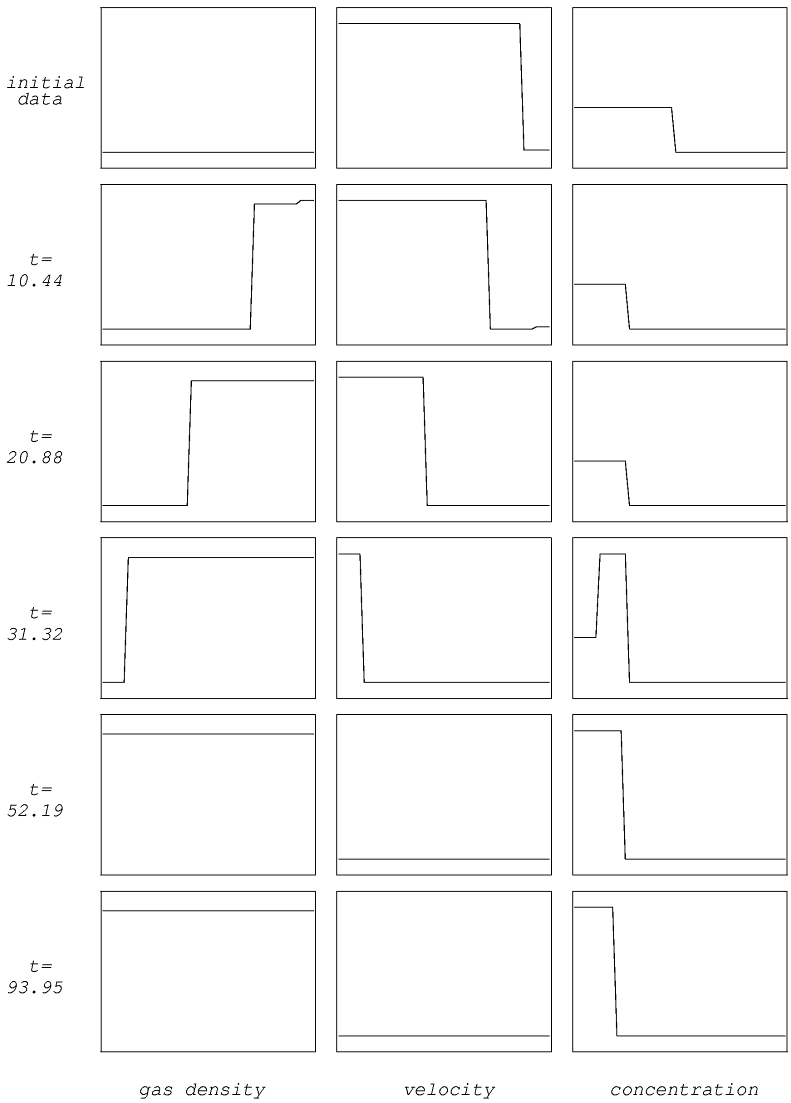

Figure 2. Example of evolution of two consecutive Riemann problems
(initial data: $v_L=2.5$, $v_R=0$, $w_{AL}=0.4$, $w_{AR}=0$ and constant r)

Figures 1 and 2 show results for the mass density r, the velocity v and the pollutant concentration per unit mass rw_A (illustrating a combination of the behavior of both r and w_A), considering the two consecutive Riemann problems solved in the present work. In all depicted sketches the right-hand side of the rectangle represents the impermeable wall of the semi-infinite region and six distinct time instants are presented, the first one showing the initial data. In Figure 1 the initial data presents a jump for both velocity v and pollutant concentration w_A with $v_L > v_R$ and $w_{AL} < w_{AR}$. Besides, both jumps have been imposed at the same spatial position in the initial condition. In figure 2 the same above described behavior is imposed for the velocity field, while the jump imposed for pollutant concentration w_A as initial data is placed at a larger distance from the impermeable wall (compared to the jump imposed for the velocity) with $w_{AL} > w_{AR}$.

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