



ONEDIMENSIONAL SIMULATION OF POLLUTANT TRANSPORT IN AN ATMOSPHERE WITH A DISCONTINUOUS MASS DENSITY

Flávia Cristina Petersen¹ and Maria Laura Martins-Costa²

Laboratory of Theoretical and Applied Mechanics - LMTA
Mechanical Engineering Department - Universidade Federal Fluminense
Rua Passo da Pátria, 156 -- 24210-240 Niterói/RJ, Brazil
E-mail: ⁽¹⁾flaviapetersen@ig.com.br / ⁽²⁾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
E-mail: rsgama@domain.com.br

***Abstract.** In this work, the transport of a pollutant in the atmosphere is modeled as a nonlinear system of hyperbolic equations, which admits discontinuities in addition to smooth or classical solutions. The equations include mass and linear momentum conservation for the air-pollutant mixture as well as the mass balance for the pollutant. The main subject in this work is the Riemann problem associated with a class of problems describing the transport of a pollutant in an ideal gas with constant temperature with a discontinuous mass density distribution as initial condition, whose solution is discussed.*

***Keywords:** Pollutant transport, isothermal atmosphere, Riemann problem, discontinuous mass density, generalized solution.*

1. INTRODUCTION

Modeling of most transport phenomena usually gives rise to parabolic or elliptic partial differential equations. Such mathematical descriptions always admit regular solutions whose simulation may employ well known numerical procedures such as finite elements, finite differences or finite volumes.

In this work the mathematical model gives rise to a nonlinear system of hyperbolic equations: the equations describing the transport of a pollutant in the air which consider, besides mass and linear momentum conservation for the air-pollutant mixture – the classical equations of gas dynamics – the mass balance for the pollutant. Like the Euler equations in gas dynamics, the system modeling the transport of a pollutant in the air is composed by a set of nonlinear hyperbolic equations, which admit discontinuities in addition to smooth or classical solutions.

The mathematical description gives rise to a set of three coupled nonlinear differential equations: a genuinely nonlinear hyperbolic problem with a very interesting feature – a contact shock characterized by the absence of entropy increase – associated with the second eigenvalue. Along this shock there is a jump in the pollutant concentration, but, on the other hand, the mass density and the velocity remain constant, i.e. they do not jump.

The main subject of this article is the Riemann problem associated with a class of problems describing the transport of a pollutant in an ideal gas with constant temperature, whose solution is

¹ This author is a graduate student at Mechanical Engineering Program (PGMEC)/UFF.

² All article correspondence should be addressed to this author.

discussed. The Riemann problem treated in the present work consists of a hyperbolic initial value problem subjected to a step function characterizing a discontinuous mass density distribution as initial data, which admits analytical generalized solution.

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:

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

in which \mathbf{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, \mathbf{w}_A , is defined as the mass fraction of this constituent in the mixture, being expressed by the following equation $\mathbf{w}_A \equiv \mathbf{r}_A / \mathbf{r}$. 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 – \mathbf{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:

$$\begin{aligned} \frac{\partial \mathbf{r}}{\partial t} + \nabla \cdot (\mathbf{r} \mathbf{v}) &= 0 \\ \frac{\partial (\mathbf{r} \mathbf{v})}{\partial t} + \nabla \cdot (\mathbf{r} \mathbf{v} \mathbf{v}) &= -\nabla p + \mathbf{r} \mathbf{g} \\ \frac{\partial (\mathbf{r} \mathbf{w}_A)}{\partial t} + \nabla \cdot (\mathbf{r} \mathbf{w}_A \mathbf{v}) &= \nabla \cdot (\mathbf{r} D \nabla \mathbf{w}_A) + r_A \end{aligned} \quad (2)$$

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 \mathbf{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 \mathbf{r} only, its derivative with respect to \mathbf{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:

$$\begin{aligned} \frac{\partial \mathbf{r}}{\partial t} + \frac{\partial}{\partial x}(\mathbf{r}v) &= 0 & \frac{\partial \mathbf{r}}{\partial t} + \frac{\partial(\mathbf{r}v)}{\partial x} &= 0 \\ \frac{\partial}{\partial t}(\mathbf{r}v) + \frac{\partial}{\partial x}(\mathbf{r}v^2 + p) &= 0 & \frac{\partial(\mathbf{r}v)}{\partial t} + \frac{\partial(\mathbf{r}v^2)}{\partial x} + p' \frac{\partial \mathbf{r}}{\partial x} &= 0 \\ \frac{\partial}{\partial t}(\mathbf{r}w_A) + \frac{\partial}{\partial x}(\mathbf{r}w_A v) &= 0 & \frac{\partial(\mathbf{r}w_A)}{\partial t} + \frac{\partial(\mathbf{r}w_A v)}{\partial x} &= 0 \end{aligned} \quad (3)$$

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

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

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

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

3. 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 (Martins-Costa and Saldanha da Gama, 2001) is a special initial value problem defined as:

$$\frac{\partial}{\partial t} \begin{bmatrix} F \\ G \\ H \end{bmatrix} + \begin{bmatrix} 0 & 1 & 0 \\ -\frac{G^2}{F^2} + p' & 2\frac{G}{F} & 0 \\ -\frac{GH}{F^2} & \frac{H}{F} & \frac{G}{F} \end{bmatrix} \frac{\partial}{\partial x} \begin{bmatrix} F \\ G \\ H \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad \text{for } -\infty < x < +\infty, t > 0 \quad (6)$$

$$\begin{aligned}
(F, G, H) &= (F_L, G_L, H_L) & \text{for } x < 0 \text{ and } t = 0 \\
(F, G, H) &= (F_R, G_R, H_R) & \text{for } x > 0 \text{ and } t = 0
\end{aligned} \tag{7}$$

At this point it is interesting to remark that the variables \mathbf{r}, v and \mathbf{w}_A and, consequently, F, G and H , are functions of both x and t , being subject to a step function as initial condition – specified in equation (7), 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.

It can be shown that a generalized solution for the Riemann problem described in equations (6)-(7), depending on the set of variables (x, t) , may be expressed as a function of a similarity variable $\mathbf{x} = x/t$. A problem depending on the set of variables (x, t) may be converted in a problem depending solely on $\mathbf{x} = x/t$ provided that two necessary and sufficient conditions are satisfied. First the dependence on $\mathbf{x} = x/t$ requires constant values for the function both at the left-hand side and at the right-hand side, 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 ∞ :

$$\begin{aligned}
(F, G, H) &= (F_L, G_L, H_L) & \text{for } \mathbf{x} = x/t \rightarrow -\infty \\
(F, G, H) &= (F_R, G_R, H_R) & \text{for } \mathbf{x} = x/t \rightarrow +\infty
\end{aligned}$$

The second condition is that the problem must be homogeneous so that equation (3) or (5) may remain homogeneous as the dependence on both variables x and t

$$\frac{\partial}{\partial t} \begin{bmatrix} F \\ G \\ H \end{bmatrix} + \mathbf{M} \frac{\partial}{\partial x} \begin{bmatrix} F \\ G \\ H \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \text{ with } \begin{cases} (F, G, H) = (F_L, G_L, H_L) & x < 0; \quad t = 0 \\ (F, G, H) = (F_R, G_R, H_R) & x > 0; \quad t = 0 \end{cases}$$

is converted in a dependence on the similarity variable \mathbf{x} . In the above equation \mathbf{M} represents the matrix presented in equation (6). Substituting $\mathbf{x} = x/t$, the associated Riemann problem may be rewritten as

$$-\mathbf{x} \frac{d}{d\mathbf{x}} \begin{bmatrix} F \\ G \\ H \end{bmatrix} + \begin{bmatrix} 0 & 1 & 0 \\ -\frac{G^2}{F^2} + p' & 2\frac{G}{F} & 0 \\ -\frac{GH}{F^2} & \frac{H}{F} & \frac{G}{F} \end{bmatrix} \frac{d}{d\mathbf{x}} \begin{bmatrix} F \\ G \\ H \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \text{ for } -\infty < \mathbf{x} < +\infty \tag{8}$$

$$\begin{aligned}
(F, G, H) &= (F_L, G_L, H_L) & \text{for } \mathbf{x} \rightarrow -\infty \\
(F, G, H) &= (F_R, G_R, H_R) & \text{for } \mathbf{x} \rightarrow +\infty
\end{aligned} \tag{9}$$

The generalized solution of equations (8)-(9) may be employed in the simulation of the complete set of equations describing the advective-diffusive transport of a pollutant in the atmosphere, given by equation (1), or, alternatively (2) through Glimm's difference scheme (Glimm, 1965).

The first step to solve the associated Riemann problem is to compute Riemann invariants from the original eigenvalues problem, giving rise a following system that allows to determine the eigenvalues – in crescent order – corresponding to equation (8),

$$I_i = \frac{G}{F} + a_i \sqrt{p'} = v + a_i \sqrt{p'}, \quad \text{with } a_i = i - 2 \quad (10)$$

If it can be assured that $p' > 0$, for all values assumed by the similarity variable \mathbf{x} and all time instants t , then equations (8) represent a genuinely nonlinear hyperbolic system and equations (8)-(9) are called a Riemann problem. The generalized solution of this Riemann problem depends only on the ratio $\mathbf{x} = x/t$ 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: $(F_L, G_L, H_L) \rightarrow (F_{*1}, G_{*1}, H_{*1}) \rightarrow (F_{*2}, G_{*2}, H_{*2}) \rightarrow (F_R, G_R, H_R)$, in which *1 and *2 indicate intermediate constant states to be determined. The connection between the states $L \rightarrow *1$, $*1 \rightarrow *2$ and $*2 \rightarrow R$ may be performed either by rarefactions or shocks. Two states are connected by an i -Rarefaction – a continuous solution of the Riemann problem – when the corresponding eigenvalues I_i are increasing functions of $\mathbf{x} = x/t$ between these states. In this case, the solution depends continuously on \mathbf{x} between these states. On the other hand, if the eigenvalues I_i are non-increasing functions of $\mathbf{x} = x/t$, 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 $v = H / \mathbf{r}$ - 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.

A shock is a special kind of jump satisfying both the Rankine-Hugoniot jump condition and the entropy condition (Smoller, 1983). Two states are connected by an i -Shock if the eigenvalues I_i are decreasing functions of $\mathbf{x} = x/t$. In this case, the entropy conditions are automatically satisfied. Considering two given states connected by an i -Shock with speed s , the following jump conditions associated with equation (8) must be satisfied

$$s = \frac{[[\mathbf{r}v]]}{[[\mathbf{r}]]} = \frac{[[\mathbf{r}v^2 + p]]}{[[\mathbf{r}v]]} = \frac{[[\mathbf{r}v\mathbf{w}_A]]}{[[\mathbf{r}\mathbf{w}_A]]} \Rightarrow s = \frac{[[G]]}{[[F]]} = \frac{[[G^2 / F + p]]}{[[G]]} = \frac{[[GH / F]]}{[[H]]} \quad (11)$$

Equation (11) expresses the Rankine-Hugoniot jump condition, in which s represents the shock speed and $[[f]]$, the jump of the quantity f .

3.1. Jump in the Connection *1 \rightarrow *2

Considering this connection, characterized by the eigenvalue $I_2 = \frac{G}{F} = v$, the associated shock speed s – using the first equation presented in (11) which requires v to be constant when \mathbf{w}_A presents a jump – could be expressed as

$$s_2 = \frac{\llbracket \mathbf{r}v \rrbracket}{\llbracket \mathbf{r} \rrbracket} \Rightarrow s_2 = \frac{\llbracket \mathbf{r} \rrbracket v}{\llbracket \mathbf{r} \rrbracket} \Rightarrow I_2 = s_2 = v \Rightarrow \text{CONTACT SHOCK} \quad (12)$$

This allows concluding that, since $v_{*1} = v_{*2}$, there is no velocity jump between these states. Using the second equation in (11) to compute the jump, it comes that $\llbracket p \rrbracket = 0$, so there is no jump for the pressure between these states either, allowing to conclude that $\mathbf{r}_{*1} = \mathbf{r}_{*2}$, since $p = p(\mathbf{r})$. In short, there is no jump for neither the velocity nor the mass density between the given states. Thus only the mass fraction of the pollutant in the mixture, \mathbf{w}_A , may present a jump, which, according to the third equation of (11), is given by $s_2 = \frac{\llbracket \mathbf{r}v\mathbf{w}_A \rrbracket}{\llbracket \mathbf{r}\mathbf{w}_A \rrbracket} = \frac{\mathbf{r}v\llbracket \mathbf{w}_A \rrbracket}{\mathbf{r}\llbracket \mathbf{w}_A \rrbracket} = v \Rightarrow \frac{\llbracket \mathbf{w}_A \rrbracket}{\llbracket \mathbf{w}_A \rrbracket} = 1$, showing that – apart from restrictions derived from initial conditions – there are no restrictions on the jump of \mathbf{w}_A . Besides, observing equation (10), it comes that the variable \mathbf{w}_A has no influence on the eigenvalues. The absence of restrictions on the jump of \mathbf{w}_A allows the choice of $\llbracket \mathbf{w}_A \rrbracket = 0$, the connection between the states $*1 \rightarrow *2$ being characterized by $\mathbf{w}_{A*1} = \mathbf{w}_{AL}$ and $\mathbf{w}_{A*2} = \mathbf{w}_{AR}$. This allows deriving an important conclusion: the pollutant is propagated with a speed v since it is carried by the atmosphere. Finally, the connections in the Riemann problem referred in equations (8)-(9) may be summarized as

$$\begin{array}{ccccccc} L & \xRightarrow{\substack{R1 \text{ or } S1}} & *1 & \xRightarrow{\text{Contact Shock}} & *2 & \xRightarrow{\substack{R3 \text{ or } S3}} & R \\ & & \mathbf{w}_{A*1} = \mathbf{w}_{AL} & & \mathbf{w}_{A*2} = \mathbf{w}_{AR} & & \\ & & \mathbf{r}_{*1} = \mathbf{r}_{*2} = \mathbf{r}_* & & & & \\ & & v_{*1} = v_{*2} = v_* & & & & \end{array} \quad (13)$$

in which $R1$ and $R3$ denote possible rarefaction in connections 1 and 3 while $S1$ and $S3$ refer to possible shock in these connections. An important simplification is possible because of the above stated result, which allows the problem reduction to a two variables (v and \mathbf{r}) problem with only two connections to be determined, namely, $L \xRightarrow{\substack{R1 \text{ or } S1}} * \xRightarrow{\substack{R3 \text{ or } S3}} R$. So, the referred states may be

connected either by an i -Rarefaction or an i -Shock. In order to determine the connections, the first step is to assume i -Rarefaction connections – corresponding to continuous solutions, then verify if the corresponding eigenvalues I_i are increasing functions of \mathbf{x} between these states, characterizing the rarefaction-type connection. This may be achieved by substituting the eigenvalues I_1 and I_3 in the equation for the Riemann invariants, resulting in

$$v = \int \pm \sqrt{p'} \frac{d\mathbf{r}}{\mathbf{r}} \quad (14)$$

From equation (14) it can be noticed that the i -th Riemann invariant depends on the constitutive relation for the pressure as a function of the mass density. A polytropic process is characterized by the equation $p = g\mathbf{r}^n$, the i -th Riemann invariant being a function of n , an isothermal process for an ideal gas corresponding to $n=1$. For $(\bar{c})^2 = RT$,

$v = \int \pm \bar{c} \frac{d\mathbf{r}}{\mathbf{r}} = \pm \bar{c} \ln \mathbf{r} + \text{constant}$, giving rise to $v + \bar{c} \ln \mathbf{r} = C_1$, for the first Riemann invariant and $v - \bar{c} \ln \mathbf{r} = C_2$ for the third Riemann invariant.

A Rarefaction 1 is obtained by assuming constant the first Riemann invariant, namely $v + \bar{c} \ln \mathbf{r} = C_1$ must be related to the eigenvalue \mathbf{I}_1

$$\mathbf{r} = \exp \left[\frac{\bar{c} \ln \mathbf{r}_L + v_L - \bar{c} - \frac{x}{t}}{\bar{c}} \right] \quad (15)$$

Substituting \mathbf{r} previously determined in $v + \bar{c} \ln \mathbf{r} = C_1$, v may be determined

$$v = 2v_L - \bar{c} - \frac{x}{t} \quad (16)$$

A Rarefaction 3 is obtained by assuming constant the third Riemann invariant, namely $v + \bar{c} \ln \mathbf{r} = C_2$ must be related to the eigenvalue \mathbf{I}_3 , so that:

$$\mathbf{r} = \exp \left[\frac{\bar{c} \ln \mathbf{r}_R - v_R - \bar{c} + \frac{x}{t}}{\bar{c}} \right] \quad \text{and} \quad v = 2v_R + \bar{c} - \frac{x}{t} \quad (17)$$

At this point it is important to observe that the equality $\mathbf{I} = x/t$ 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 are functions with jump conditions satisfying the Rankine-Hugoniot condition stated in equation (11).

It is important to bear 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, indicating that the entropy of the correct solution must be increased as the solution crosses a shock. In short, when two states are connected by a shock, with speed s_i , the jump conditions associated with the Riemann problem stated in equation (8) must be satisfied.

4. DETERMINATION OF THE CONNECTION BETWEEN THE STATES

The determination of the type of connection requires the representation of Riemann invariants as functions of the eigenvalues. These invariants may be expressed as:

$$\mathfrak{R}_1 = \underbrace{\mathbf{I}_1 + \sqrt{p'}}_v + \underbrace{\int \frac{\sqrt{p'}}{\mathbf{r}} d\mathbf{r}}_f \quad \text{and} \quad \mathfrak{R}_3 = \underbrace{\mathbf{I}_3 - \sqrt{p'}}_v - \underbrace{\int \frac{\sqrt{p'}}{\mathbf{r}} d\mathbf{r}}_f \quad (18)$$

Making $\mathbf{y}(\mathbf{r}) = \sqrt{p'} + \int \frac{\sqrt{p'}}{\mathbf{r}} d\mathbf{r}$ since $p = \hat{p}(\mathbf{r})$ it comes that $\mathfrak{R}_1 = \mathbf{I}_1 + \mathbf{y}(\mathbf{r})$ and $\mathfrak{R}_3 = \mathbf{I}_3 - \mathbf{y}(\mathbf{r})$. If $\mathbf{I}_{1L} < \mathbf{I}_{1*}$ the connection is a 1-Rarefaction, but since $\mathbf{I}_{1L} + \mathbf{y}_L(\mathbf{r}) = \mathbf{I}_{1*} + \mathbf{y}_*(\mathbf{r})$, then $\mathbf{I}_{1L} - \mathbf{I}_{1*} = \mathbf{y}_*(\mathbf{r}) - \mathbf{y}_L(\mathbf{r})$, allowing to conclude that $\Rightarrow \mathbf{I}_{1L} < \mathbf{I}_{1*} \Leftrightarrow \mathbf{y}_*(\mathbf{r}) < \mathbf{y}_L(\mathbf{r})$ and if

$I_{3^*} < I_{3R}$ the connection is a 3-Rarefaction, but since $I_{3^*} - \mathbf{y}_*(\mathbf{r}) = I_{1R} + \mathbf{y}_R(\mathbf{r})$, then $I_{3^*} - I_{3R} = \mathbf{y}_*(\mathbf{r}) - \mathbf{y}_R(\mathbf{r})$, allowing to conclude that $\Rightarrow I_{3^*} < I_{3R} \Leftrightarrow \mathbf{y}_*(\mathbf{r}) < \mathbf{y}_R(\mathbf{r})$. So, for connections 1-Rarefaction – 3-Rarefaction, it can be concluded, simultaneously, that $\mathbf{y}_*(\mathbf{r}) < \mathbf{y}_L(\mathbf{r})$ and $\mathbf{y}_*(\mathbf{r}) < \mathbf{y}_R(\mathbf{r})$. But, since $p = \mathbf{g}\mathbf{r}^n$ with $n \geq 1$, $\mathbf{y}(\mathbf{r})$ increases as \mathbf{r} increases.

5. SOME RESULTS

In order to illustrate the theory presented in the last section, the particular situation in which at a given time (usually $t=0$) the velocity is zero everywhere while there is a jump in both the mass density and the concentration fields at the point $x=0$ is now considered.

This problem illustrates the interaction mechanism between two atmospheres, separated by an impermeable surface until a given instant $t=0$, suddenly exposed to one another at a time $t>0$, giving rise to a non-equilibrium situation.

The jump of the field \mathbf{r} at a time $t>0$ gives rise to a motion in a sense of reaching an equilibrium situation. So, assuming $\mathbf{r}_L > \mathbf{r}_R$, a positive velocity v_* arises in the vicinity of the point $x=0$, this vicinity being enlarged as t increases. Since the second eigenvalue is given by v_* , the position of the jump of the concentration \mathbf{w}_A moves from left to right with a velocity v_* .

In the region where the velocity is given by v_* , the mass density is given by \mathbf{r}_* , being $\mathbf{r}_* < \mathbf{r}_L$ and $\mathbf{r}_* > \mathbf{r}_R$, simultaneously. This allows concluding that the concentration per unit mass $\mathbf{r}\mathbf{w}_A$ is not a step function as the concentration \mathbf{w}_A .

These comments are based on a generalized solution composed by a 1-Rarefaction, a 3-Shock and a 2-(Contact)-Shock, for the particular situation described in the first paragraph. The 1-Rarefaction provides a continuous connection between $(\mathbf{r}_L, v_L=0)$ and (\mathbf{r}_*, v_*) , usually falling in the left side of plane $x-t$. The region of 1-Rarefaction is defined by $-\bar{c} < x/t < v_* - \bar{c}$

Between $(\mathbf{r}_R, v_R=0)$ and (\mathbf{r}_*, v_*) , there is a shock with positive speed s_3 given by $\mathbf{r}_*v_*/(\mathbf{r}_* - \mathbf{r}_R)$.

The contact shock with speed $s_2 = I_2 = v_*$ is associated with the jump in the concentration \mathbf{w}_A only. For $x/t < s_2$, $\mathbf{w}_A = \mathbf{w}_{AL}$ while for $x/t > s_2$, $\mathbf{w}_A = \mathbf{w}_{AR}$.

Taking into account that $v_L = v_R = 0$, the velocity v_* and the mass density \mathbf{r}_* may be determined from the following system:

$$\begin{cases} 0 + \bar{c} \ln \mathbf{r}_L = v_* + \bar{c} \ln \mathbf{r}_* \\ v_* = \sqrt{\left(\frac{1}{\mathbf{r}_R} - \frac{1}{\mathbf{r}_*}\right) \bar{c}^2 (\mathbf{r}_* - \mathbf{r}_R)} \end{cases} \quad (19)$$

Table 1. Results for intermediate states

\mathbf{r}_L	\mathbf{r}_R	\mathbf{r}_*	$u_* = v_* / \bar{c}$
1.00000	1.00000	1.00000	0.00000
2.00000	1.00000	1.41299	0.49092
3.00000	1.00000	1.72617	0.95407
4.00000	1.00000	1.98649	1.39039
5.00000	1.00000	2.21267	1.80385
6.00000	1.00000	2.41445	2.19784
7.00000	1.00000	2.59769	2.57506

\mathbf{r}_L	\mathbf{r}_R	\mathbf{r}_*	$u_* = v_* / \bar{c}$
8.00000	1.00000	2.76624	2.93762
9.00000	1.00000	2.92278	3.28722
10.00000	1.00000	3.06928	3.62526
2.00000	2.00000	2.00000	0.00000
3.00000	2.00000	2.44907	0.99386
4.00000	2.00000	2.82599	1.96370
5.00000	2.00000	3.15601	2.90434
6.00000	2.00000	3.45234	3.81627
7.00000	2.00000	3.72291	4.70132
8.00000	2.00000	3.97299	5.56157
9.00000	2.00000	4.20623	6.39900
10.00000	2.00000	4.42534	7.21541
3.00000	3.00000	3.00000	0.00000
4.00000	3.00000	3.46389	1.49539
5.00000	3.00000	3.87164	2.97062
6.00000	3.00000	4.23898	4.41832
7.00000	3.00000	4.57539	5.83662
8.00000	3.00000	4.88710	7.22571
9.00000	3.00000	5.17851	8.58661
10.00000	3.00000	5.45283	9.92061
4.00000	4.00000	4.00000	0.00000
5.00000	4.00000	4.47201	1.99632
6.00000	4.00000	4.89813	3.97544
7.00000	4.00000	5.28910	5.92934
8.00000	4.00000	5.65198	7.85480
9.00000	4.00000	5.99174	9.75078
10.00000	4.00000	6.31203	11.61736
5.00000	5.00000	5.00000	0.00000
6.00000	5.00000	5.47714	2.49693
7.00000	5.00000	5.91549	4.97893
8.00000	5.00000	6.32285	7.43793
9.00000	5.00000	6.70467	9.86995
10.00000	5.00000	7.06497	12.27312
6.00000	6.00000	6.00000	0.00000
7.00000	6.00000	6.48068	2.99737
8.00000	6.00000	6.92777	5.98156
9.00000	6.00000	7.34720	8.94473
10.00000	6.00000	7.74329	11.88248
7.00000	7.00000	7.00000	0.00000
8.00000	7.00000	7.48327	3.49770
9.00000	7.00000	7.93693	6.98362
10.00000	7.00000	8.36561	10.45022
8.00000	8.00000	8.00000	0.00000
9.00000	8.00000	8.48525	3.99796
10.00000	8.00000	8.94401	7.98526
9.00000	9.00000	9.00000	0.00000
10.00000	9.00000	9.48680	4.49817
10.00000	10.00000	10.00000	0.00000

Table 1 shows results for an intermediate state (*). It is important to notice that the motion is caused by the jump in the mass density, so that if $\mathbf{r}_L = \mathbf{r}_R$ it comes that $u_* = 0$, i.e., there is no motion. Figure 1 presents results for three fields, namely the mass density \mathbf{r} , the velocity v and the pollutant concentration per unit mass $\mathbf{r}\mathbf{w}_A$ (illustrating a combination of the behavior of both \mathbf{r} and \mathbf{w}_A) as a function of x for six distinct time instants, the first one showing discontinuous initial data where $\mathbf{w}_{AL} > \mathbf{w}_{AR}$ and $\mathbf{r}_L > \mathbf{r}_R$. In the five subsequent time instants the shocks may be clearly observed at the right-hand side, as well as the continuous solution at the left-hand side.

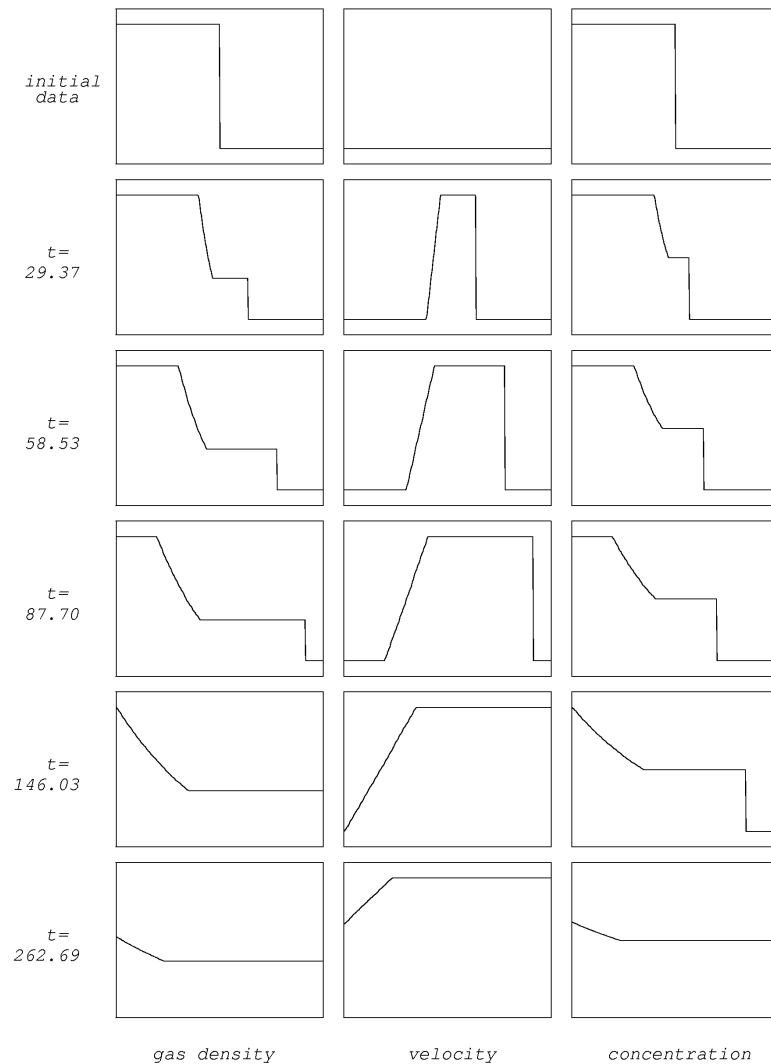


Figure 1. Example of evolution of Riemann problem

6. ACKNOWLEDGMENTS

The authors F.C. Petersen, M.L. Martins-Costa and R.M. Saldanha da Gama gratefully acknowledge the financial support provided by the Brazilian agencies CAPES through grant PGMEC/UFF and CNPq through grants 300404/91-3 and 302462/84-8, respectively.

7. REFERENCES

- Glimm, J., 1965, "Solutions in the Large for Nonlinear Hyperbolic Systems of Equations", Communications in Pure and Applied Mathematics, Vol. 18, pp. 697-715.
- John, F., 1982, "Partial Differential Equations", Springer Ed., Berlin, Germany, 428 p.
- Martins-Costa, M.L. and Saldanha da Gama, R.M., 2001, "Numerical Simulation of One-dimensional Flows through Porous Media with Shock Waves", International Journal for Numerical Methods in Engineering, Vol. 52, pp. 1047-1067.
- Smoller, J., 1983, "Shock-Waves and Reaction-Diffusion Equations", Springer Ed., Berlin, Germany, 428 p.