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A mathematical model and a numerical model for hyperbolic mass transport in compressible flows

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Abstract A number of contributions have been made during the last decades to model pure-diffusive transport problems by using the so-called *hyperbolic diffusion equations*. These equations are used for both mass and heat transport. The hyperbolic diffusion equations are obtained by substituting the classic constitutive equation (Fick's and Fourier's law, respectively), by a more general differential equation, due to Cattaneo (C R Acad Sci Ser I Math 247:431–433, 1958). In some applications the use of a parabolic model for diffusive processes is assumed to be accurate enough in spite of predicting an infinite speed of propagation (Cattaneo, C R Acad Sci Ser I Math 247:431–433, 1958). However, the use of a wave-like equation that predicts a finite velocity of propagation is necessary in many other calculations. The studies of heat or mass transport with finite velocity of propagation have been traditionally limited to pure-diffusive situations. However, the authors have recently proposed a generalization of Cattaneo's law that can also be used in convective-diffusive problems (Gómez, Technical Report (in Spanish), University of A Coruña, 2003; Gómez et al., in An alternative formulation for the advective-diffusive transport problem. 7th Congress on computational methods in engineering. Lisbon, Portugal, 2004a; Gómez et al., in On the intrinsic instability of the advection–diffusion equation. Proc. of the 4th European congress on computational methods in applied sciences and engineering (CDROM). Jyväskylä, Finland, 2004b) (see also Christov and Jordan, Phys Rev Lett 94:4301–4304, 2005). This constitutive equation has been applied to engineering problems in the context of mass transport within an incompressible fluid (Gómez et al., Comput Methods Appl Mech Eng, doi:10.1016/j.cma.2006.09.016, 2006). In this paper we extend the model to compressible flow problems. A discontinuous Galerkin method is also proposed to numerically solve the equations. Finally, we present some examples to test out the performance of the numerical and the mathematical model.

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1 Introduction

There is much experimental evidence which proves that diffusive processes take place with finite velocity inside matter [1, 2]. In some applications, this issue can be ignored and the use of Fick's [3] law or Fourier's [4] law (in the case of mass transport or heat conduction, respectively), is assumed to be accurate enough for practical purposes in spite of predicting an infinite speed of propagation. However, in many other instances [5] it is necessary to take into account the wave nature of diffusive processes to perform accurate predictions. This kind of approach cannot be carried out by using Fick's law or Fourier's law [1, 6]. Instead a more general constitutive law, for example the one proposed by Cattaneo [7], must be employed.

A great deal of effort has been devoted to the study of hyperbolic diffusion (see [8, 9] for a detailed state of the art in this topic) and Cattaneo's law is still the most widely accepted model for diffusive processes. However, there is also some criticism to Cattaneo's law (see, for instance, [10–14]).

Due to the practical interest of the hyperbolic pure-diffusion equation, some numerical models have been developed for the approximation of its solution. The numerical simulation of the hyperbolic diffusion equations has been mostly limited to 1D problems (see for instance [10, 15–17]). The numerical discretization of 2D pure-diffusion problems was probably pioneered by Yang [18]. Later, Manzari and Manzari [19] proposed a different algorithm and solved some practical pure-diffusive examples. More recently Shen and Han [20] have solved the 2D hyperbolic pure-diffusion equation with non-linear boundary conditions.

This paper deals with problems of mass transport within a fluid. In the context of many engineering applications it is important to consider both, diffusion and convection, phenomena since none of these transport processes can be ignored. For this reason, the authors have recently proposed a generalization of Cattaneo's law that can also be used in convective-diffusive problems [21–23]. This equation was applied to the resolution of practical problems in the context of mass transport within an incompressible fluid [24]. In this paper we extend the model to compressible flow problems. A discontinuous Galerkin method is proposed to solve numerically the equations. Finally, we present some examples to test out the numerical and the mathematical models.

The outline of this paper is as follows: in Sect. 2 we derive the proposed equations for the description of mass transport within a compressible fluid. In Sect. 3 we study the main properties of the proposed model. A discontinuous Galerkin method to solve numerically the proposed equations is introduced in Sect. 4. Section 5 is devoted to the presentation of some numerical examples. Finally, Sect. 6 gathers the main conclusions of this study.

2 Governing equations

The use of a hyperbolic model to describe pure-diffusive phenomena has been addressed with increasing interest in last years. The governing equations for this kind of models have been normally obtained by using a generalized form of Fick's law that was first proposed by Cattaneo [7]. Cattaneo's equation in 1D takes the form

$$f + \tau \frac{\partial f}{\partial t} = -k\rho \frac{\partial \lambda}{\partial x} \tag{1}$$

where λ is the pollutant concentration, f is the pollutant flux, ρ is the fluid density and k is the diffusivity. Cattaneo's equation introduces the concept of *relaxation time* τ which plays the role of an "inertia" for the movement of the pollutant. Equation (1) can be closed by using the mass conservation equations (conservation of pollutant mass and conservation of fluid mass). By doing so, we obtain a totally hyperbolic system of partial differential equations where

$$c_c = \sqrt{k/\tau}. \tag{2}$$

is the velocity of propagation. The aforementioned system governs the phenomenon of the hyperbolic pure-diffusion. However, we are interested in applying Cattaneo's ideas to those problems that involve convective transport, as well [21–23]. For this reason, we have recently proposed [21] the following constitutive equation

$$\boldsymbol{f} + \boldsymbol{\tau} \frac{D\boldsymbol{f}}{Dt} = -\boldsymbol{K}\rho \nabla_x(\lambda) \tag{3}$$

where

$$\frac{D\boldsymbol{f}}{Dt} = \frac{\partial \boldsymbol{f}}{\partial t} + \nabla_x(\boldsymbol{f})\, \boldsymbol{v}, \tag{4}$$

$\boldsymbol{\tau}$ is the so-called relaxation tensor and $\boldsymbol{K}$ is the diffusivity tensor. Equation (3) may be used when the medium is moving with velocity $\boldsymbol{v}$. It has been derived from Cattaneo's law by imposing Galilean invariance principle to the resulting model. In this way, the description of the diffusion process is granted to be the same in every inertial frame [25].

We are interested in applying Eq. (3) to mass transport problems in compressible fluids. In order to formulate the problem we also have to use the fluid dynamics equations and the pollutant mass conservation equation. Taking into account all of this, the governing equations can be written as:

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho \boldsymbol{v}) = 0 \tag{5.1}$$

$$\frac{\partial (\rho \boldsymbol{v})}{\partial t} + \nabla_x \cdot (\rho \boldsymbol{v} \otimes \boldsymbol{v} + p\boldsymbol{I} - \mathcal{T}) = 0 \tag{5.2}$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla_x \cdot (H\boldsymbol{v} - \mathcal{T}\boldsymbol{v}) = 0 \tag{5.3}$$

$$\frac{\partial (\rho \lambda)}{\partial t} + \nabla_x \cdot (\rho \lambda \boldsymbol{v} + \boldsymbol{f}) = 0 \tag{5.4}$$

$$\boldsymbol{f} + \boldsymbol{\tau}\left(\frac{\partial \boldsymbol{f}}{\partial t} + \nabla_x(\boldsymbol{f})\boldsymbol{v}\right) = -\boldsymbol{K}\rho \nabla_x(\lambda) \tag{5.5}$$

where p represents the pressure and $\boldsymbol{v}$ is the fluid velocity. The total energy and the enthalpy are given by

$$\rho E = \rho e + \frac{1}{2}\rho \boldsymbol{v} \cdot \boldsymbol{v}; \quad H = E + \frac{p}{\rho} \tag{6}$$

where e is the specific internal energy. The viscous stresses are modeled as

$$\mathcal{T} = \mu\left(\nabla_x(\boldsymbol{v}) + \nabla_x(\boldsymbol{v})^T - \frac{2}{3}\nabla_x \cdot (\boldsymbol{v})\boldsymbol{I}\right) \tag{7}$$

where μ is the viscosity. The equation of state and temperature for an ideal gas can be written as

$$p = (\gamma - 1)\left(\rho E - \frac{1}{2}\rho \boldsymbol{v}\cdot\boldsymbol{v}\right); \quad T = \frac{1}{C_v}\frac{p}{\rho(\gamma-1)} \tag{8}$$

being C_v the specific heat at constant volume ($C_v = 716.5$ for air) and $\gamma = C_p/C_v$ is the ratio of specific heats ($\gamma = 1.4$ for air). Finally, the speed of sound is given by

$$c_s = \sqrt{\gamma p/\rho} \tag{9}$$

3 Study of the proposed model

With the aim of simplifying the exposition, we will consider from here on a 2D domain. The notation $\boldsymbol{v}^T = (u, v)$, $\boldsymbol{f}^T = (f_x, f_y)$ will be used.

In order to study the properties of system (5) it would be very useful to write it in conservative form. We have formulated the model by selecting two different sets of unknowns $\boldsymbol{U}$ and $\boldsymbol{U}'$, namely

$$\boldsymbol{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho\lambda \\ q_x \\ q_y \end{pmatrix}; \quad \boldsymbol{U}' = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho\lambda \\ f_x \\ f_y \end{pmatrix} \tag{10}$$

where the variable $\boldsymbol{q} = \boldsymbol{f}/\rho$ has been introduced. None of these sets of values lead to a fully conservative form of the equations. However, if variables $\boldsymbol{U}$ are selected, system (5) can be written (after non-trivial analytic work and under the assumption of homogeneous and isotropic diffusivity and relaxation time) in a very interesting form, namely

$$\frac{\partial\rho}{\partial t} + \nabla_x\cdot(\rho\boldsymbol{v}) = 0 \tag{11.1}$$

$$\frac{\partial(\rho\boldsymbol{v})}{\partial t} + \nabla_x\cdot(\rho\boldsymbol{v}\otimes\boldsymbol{v} + p\boldsymbol{I} - \mathcal{T}) = 0 \tag{11.2}$$

$$\frac{\partial(\rho E)}{\partial t} + \nabla_x\cdot(H\boldsymbol{v} - \mathcal{T}\boldsymbol{v}) = 0 \tag{11.3}$$

$$\frac{\partial(\rho\lambda)}{\partial t} + \nabla_x\cdot(\rho\lambda\boldsymbol{v} + \rho\boldsymbol{q}) = 0 \tag{11.4}$$

$$\frac{\partial\boldsymbol{q}}{\partial t} + \nabla_x\cdot(\boldsymbol{q}\otimes\boldsymbol{v} + c_c^2\lambda\boldsymbol{I}) = \left(-\frac{1}{\tau} + 2\nabla_x\cdot(\boldsymbol{v})\right)\boldsymbol{q} \tag{11.5}$$

If the right hand side of Eq. (11.5) is treated as a source term, the velocities of propagation that are found in the inviscid counterpart of system (11) are those that result of adding up the fluid velocity to the speed of sound and to the pollutant velocity [see Eqs. (18)]. For this reason we will formulate the problem taking $\boldsymbol{U}$ as the unknown.

From here on we will neglect the viscous part of system (11) to compute the fluid dynamics problem. Taking into account this hypothesis, system (11) is rewritten as

$$\frac{\partial\boldsymbol{U}}{\partial t} + \nabla_x\cdot(\boldsymbol{F}) = \boldsymbol{S} \tag{12}$$

where vector $\boldsymbol{S}$ and the flux matrix $\boldsymbol{F}$ take the form

$$\boldsymbol{F} = \begin{pmatrix} \rho u & \rho v \\ \rho u^2 + p & \rho uv \\ \rho uv & \rho v^2 + p \\ \rho H u & \rho H v \\ \rho\lambda u + \rho q_x & \rho\lambda v + \rho q_y \\ q_x u + \lambda c_c^2 & q_x v \\ q_y u & q_y v + \lambda c_c^2 \end{pmatrix}; \quad \boldsymbol{S} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ (-\frac{1}{\tau} + 2\nabla_x\cdot(\boldsymbol{v}))q_x \\ (-\frac{1}{\tau} + 2\nabla_x\cdot(\boldsymbol{v}))q_y \end{pmatrix} \tag{13}$$

In order to study the basic properties of system (12) it is necessary to rewrite it in a non-conservative form. In this way, if we define $\boldsymbol{F}_x$ ($\boldsymbol{F}_y$, respectively), as the first (second, respectively), column of matrix $\boldsymbol{F}$, the following relation holds:

$$\nabla_x\cdot(\boldsymbol{F}) = \frac{\partial\boldsymbol{F}_x}{\partial x} + \frac{\partial\boldsymbol{F}_y}{\partial y} = \boldsymbol{A}_x\frac{\partial\boldsymbol{U}}{\partial x} + \boldsymbol{A}_y\frac{\partial\boldsymbol{U}}{\partial y} \tag{14}$$

being $\boldsymbol{A}_x$ and $\boldsymbol{A}_y$ the Jacobian matrices defined by $\boldsymbol{A}_x = \nabla_{\boldsymbol{U}}(\boldsymbol{F}_x)$; $\boldsymbol{A}_y = \nabla_{\boldsymbol{U}}(\boldsymbol{F}_y)$.

Matrices $\boldsymbol{A}_x$ and $\boldsymbol{A}_y$ take the form

$$\boldsymbol{A}_x = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -u^2 + \frac{\gamma-1}{2}(u^2+v^2) & (3-\gamma)u & -(\gamma-1)v & \gamma-1 & 0 & 0 & 0 \\ -uv & v & u & 0 & 0 & 0 & 0 \\ u(\gamma E - 2H) & H - (\gamma-1)u^2 & -(\gamma-1)uv & \gamma u & 0 & 0 & 0 \\ q_x - \lambda u & \lambda & 0 & 0 & u & \rho & 0 \\ -(q_x u + c_c^2\lambda)/\rho & q_x/\rho & 0 & 0 & c_c^2/\rho & u & 0 \\ -q_y u/\rho & q_y/\rho & 0 & 0 & 0 & 0 & u \end{pmatrix} \tag{15}$$

$$\boldsymbol{A}_y = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -uv & v & u & 0 & 0 & 0 & 0 \\ \frac{\gamma-1}{2}(u^2+v^2)-v^2 & (1-\gamma)u & (3-\gamma)v & \gamma-1 & 0 & 0 & 0 \\ v(\gamma E-2H) & (1-\gamma)uv & -v^2(\gamma-1)+H & \gamma u & 0 & 0 & 0 \\ q_y-\lambda v & 0 & \lambda & 0 & v & 0 & \rho \\ -q_x v/\rho & 0 & q_x/\rho & 0 & 0 & v & 0 \\ -(q_y v+c_c^2\lambda)/\rho & 0 & q_y/\rho & 0 & c_c^2/\rho & 0 & v \end{pmatrix} \tag{16}$$

Now, we define the vector of matrices $\boldsymbol{A}^T = (\boldsymbol{A}_x, \boldsymbol{A}_y)$. Let $\boldsymbol{\kappa}^T = (\kappa_x,\ \kappa_y)$ be an arbitrary vector with the constriction $||\boldsymbol{\kappa}|| = 1$, where $\|\cdot\|$ denotes the Euclidean norm of a given vector. It can be shown that the equation

$$\det(\omega \boldsymbol{I} - \boldsymbol{A}\cdot\boldsymbol{\kappa}) = 0 \tag{17}$$

yields seven real solutions ω for arbitrarily prescribed values of $\boldsymbol{\kappa}$. More specifically, the solutions of (17) are

$$\omega_1 = \boldsymbol{v}\cdot\boldsymbol{\kappa} \tag{18.1}$$

$$\omega_2 = \boldsymbol{v}\cdot\boldsymbol{\kappa} \tag{18.2}$$

$$\omega_3 = \boldsymbol{v}\cdot\boldsymbol{\kappa} \tag{18.3}$$

$$\omega_4 = \boldsymbol{v}\cdot\boldsymbol{\kappa} + c_s \tag{18.4}$$

$$\omega_5 = \boldsymbol{v}\cdot\boldsymbol{\kappa} - c_s \tag{18.5}$$

$$\omega_6 = \boldsymbol{v}\cdot\boldsymbol{\kappa} + c_c \tag{18.6}$$

$$\omega_7 = \boldsymbol{v}\cdot\boldsymbol{\kappa} - c_c \tag{18.7}$$

The values written in (18) are the eigenvalues of $\boldsymbol{A}\cdot\boldsymbol{\kappa}$ which is usually called *projection matrix*. These values represent the velocities of the waves that constitute the solution of (12). These velocities correspond to the sum of the velocity pressure wave and the velocity of the pollutant wave to the fluid velocity.

A detailed observation of the velocities given by (18) allows us to conclude that the behavior of the solution is determined by two non-dimensional numbers: the first one is the so-called Mach number [26], namely

$$M = \frac{||\boldsymbol{v}||}{c_s} \tag{19}$$

The second non-dimensional number is

$$H = \frac{||\boldsymbol{v}||}{c_c} \tag{20}$$

The H number has been introduced by the authors in [21, 23] and it represents the ratio of the fluid velocity to the pollutant velocity.

It is well known that the definition of the Mach number allows classifying the flow as follows:

- $M < 1 \Leftrightarrow$ Subsonic flow
- $M > 1 \Leftrightarrow$ Supersonic flow

In subsonic flow conditions, pressure waves travel at a greater speed than the fluid does. However, in supersonic flow conditions pressure waves propagate slower than the fluid. As a consequence, pressure waves can only travel downstream in supersonic flow.

The definition of the H number also allows classifying the flow as

- $H < 1 \Leftrightarrow$ Subcritical flow
- $H > 1 \Leftrightarrow$ Supercritical flow

In subcritical flow the pollutant can travel downstream as well as upstream. However, in supercritical flow conditions the pollutant can only travel downstream. This is an important feature of the proposed model.

4 Numerical discretization of the proposed model

In this section we propose a numerical method to solve system (12). The proposed scheme is based on the discontinuous Galerkin (DG in what follows) method that is being increasingly used for the numerical approximation of hyperbolic systems. In the same way as traditional finite volume methods, the use of the DG scheme requires the definition of *numerical fluxes* across the interfaces of the elements. In this paper we propose a new numerical flux to be used in the resolution of system (12).

4.1 Discontinuous Galerkin method

The DG method is usually attributed to [27]. Since its introduction in the framework of transport of neutrons in 1973, DG methods have evolved in a manner that made them suitable for computational fluid dynamics [28]. The present popularity of the method is mainly due to Cockburn and Shu (with several collaborators) who introduced the Runge–Kutta Discontinuous Galerkin Method [29–32]. The main characteristic of the DG method is that the numerical solution is allowed to be discontinuous across the interfaces of the elements.

Whereas the continuous finite element methods were initially developed for elliptic equations, the DG method was primarily applied to hyperbolic problems. However, in

the last decade, there has been extensive research into parabolic and elliptic DG methods [33–38]

In this section a DG method for the resolution of system (12) is presented. The formulation is identical for 2D and 3D problems. From here on, we will restrict to the 2D problem in order to simplify the exposition.

Let Ω^h be a partition of the computational domain Ω into a mesh of *nelem* elements. Let Ω_{ielem} be a general element with boundary Γ_{ielem}. We also define the following space of polynomials

$$\mathcal{V}^h = \{v^h \in \mathcal{L}^2(\Omega) : v^h|_{\Omega_{ielem}} \in \mathcal{P}^m(\Omega_{ielem}), \forall \Omega_{ielem} \in \Omega^h\} \tag{21}$$

where $\mathcal{P}^m(\Omega_{ielem})$ is the space of polynomials of degree at most m. Note that the discrete space does not enforce $\mathcal{C}^0$ continuity and that m, in general, can vary in all elements. Taking into account all of this, we can derive the variational formulation of the problem by multiplying the governing equation with a smooth test function w and by integrating over the local element Ω_{ielem}

$$\iint_{\Omega_{ielem}} w\frac{\partial \boldsymbol{U}}{\partial t}\mathrm{d}\Omega + \iint_{\Omega_{ielem}} \omega\nabla_x \cdot (\boldsymbol{F})\mathrm{d}\Omega = \iint_{\Omega_{ielem}} w\boldsymbol{S}\mathrm{d}\Omega \tag{22}$$

In order to obtain the discrete Galerkin formulation we approximate $\boldsymbol{U}$ by a polynomial expansion $\boldsymbol{U}^h \in \mathcal{V}^h$. Further, we restrict the class of test functions to those $w^h \in \mathcal{V}^h$. In addition, we integrate by parts the second term in (22). By these means, we find the expression:

$$\begin{aligned}\iint_{\Omega_{ielem}} w^h\frac{\partial \boldsymbol{U}^h}{\partial t}\mathrm{d}\Omega - \iint_{\Omega_{ielem}} \boldsymbol{F}^h\nabla_x(w^h)\mathrm{d}\Omega \\ + \int_{\Gamma_{ielem}} w^h\boldsymbol{F}^h\cdot\boldsymbol{n}\mathrm{d}\Gamma = \iint_{\Omega_{ielem}} w^h\boldsymbol{S}^h\mathrm{d}\Omega\end{aligned} \tag{23}$$

Due to the discontinuous representation of the solution in the DG method, two values of the unknown $\boldsymbol{U}^h$ exist over the edges of the elements. For this reason, we substitute the discontinuous boundary flux term $\boldsymbol{F}^h\cdot\boldsymbol{n}$ for a continuous numerical flux denoted by $\widehat{\boldsymbol{F}}\cdot\boldsymbol{n}$. The numerical flux is constructed taking into account the two values of $\boldsymbol{U}^h$ that exist over the edges of each element ($\boldsymbol{U}^+$ and $\boldsymbol{U}^-$). These two values are combined in order to design the numerical flux according to the direction of propagation of the flow.

4.2 Numerical flux

As we said before, the discontinuous boundary flux term $\boldsymbol{F}^h\cdot\boldsymbol{n}$ is substituted for a continuous numerical flux $\widehat{\boldsymbol{F}}\cdot\boldsymbol{n}$. The continuous numerical flux depends on the two values of $\boldsymbol{U}^h$ that exist over the edges of the element Ω_{ielem}. We call $\boldsymbol{U}^+$ the value obtained from the element Ω_{ielem} and $\boldsymbol{U}^-$ the value obtained from its adjacent element at a given point of Γ_{ielem}.

We propose a new numerical flux to be used in the boundary term of (23). The numerical flux that we propose is of the *flux vector splitting* type. In this kind of formulations the numerical flux is written as

$$\widehat{\boldsymbol{F}}\cdot\boldsymbol{n} = \boldsymbol{F}_n^+(\boldsymbol{U}^+) + \boldsymbol{F}_n^-(\boldsymbol{U}^-) \tag{24}$$

In addition, we split $\boldsymbol{F}_n^{\pm}$ to separate the contribution that corresponds to the fluid dynamics ($\boldsymbol{F}_n^{E\pm}$) from the part related to the pollutant mass transport ($\boldsymbol{F}_n^{C\pm}$). In this way

$$\widehat{\boldsymbol{F}}\cdot\boldsymbol{n} = \boldsymbol{F}_n^{E+}(\boldsymbol{U}^+) + \boldsymbol{F}_n^{C+}(\boldsymbol{U}^+) + \boldsymbol{F}_n^{E-}(\boldsymbol{U}^-) + \boldsymbol{F}_n^{C-}(\boldsymbol{U}^-) \tag{25}$$

For the contribution that corresponds to the fluid dynamics we use a numerical flux derived from the Van Leer–Hänel flux. The Van Leer–Hänel flux corresponds to a modified form of the Van Leer scheme [39] proposed by Hänel et al. [40] for multidimensional problems [41]. Therefore, $\mathbf{F}_n^{E\pm}(\mathbf{U})$ is given by

$$\boldsymbol{F}_n^{E\pm}(\boldsymbol{U}) = \rho u_n^{\pm}\begin{pmatrix}1\\u\\v\\H\\0\\0\\0\end{pmatrix} + p^{\pm}\begin{pmatrix}0\\n_x\\n_y\\0\\0\\0\\0\end{pmatrix} \tag{26}$$

being

$$\begin{aligned}u_n^{\pm} &= \begin{cases}\pm\frac{1}{4}c_s(M_n\pm 1)^2, & |M_n|\le 1\\ \frac{1}{2}(u_n\pm|u_n|), & |M_n|>1\end{cases};\\ p^{\pm} &= \begin{cases}\frac{1}{4}p(M_n\pm 1)^2(2\mp M_n), & |M_n|\le 1\\ \frac{p}{2u_n}(u_n\pm|u_n|), & |M_n|>1\end{cases}\end{aligned} \tag{27}$$

In the previous equations it has been used the notation $u_n = \boldsymbol{v}\cdot\boldsymbol{n}$, $M_n = u_n/c_s$ and $\boldsymbol{n}^T = (n_x, n_y)$.

For the contribution that corresponds to the pollutant mass transport we propose a numerical flux based on that developed by the authors for incompressible flow computations [42, 43]. By doing so, $\boldsymbol{F}_n^{C\pm}(\boldsymbol{U})$ is given by

$$\boldsymbol{F}_n^{C\pm} = \begin{pmatrix}0\\0\\0\\0\\\frac{\rho\lambda}{4}\alpha_n^{\pm} + \frac{\rho q_n}{4c}\beta_n^{\pm}\\ \frac{\lambda c_c n_x}{4}\beta_n^{\pm} + \frac{q_x n_x^2}{4}\alpha_n^{\pm} + \frac{q_x n_y^2}{2}\gamma_n^{\pm} + \frac{q_y n_x n_y}{4}\delta_n^{\pm}\\ \frac{\lambda c_c n_y}{4}\beta_n^{\pm} + \frac{q_y n_y^2}{4}\alpha_n^{\pm} + \frac{q_y n_x^2}{2}\gamma_n^{\pm} + \frac{q_x n_x n_y}{4}\delta_n^{\pm}\end{pmatrix} \tag{28}$$

where

$$\alpha_n^{\pm} = 2u_n \pm |u_n + c_c| \pm |u_n - c_c| \tag{29.1}$$

$$\beta_n^{\pm} = 2c_c \pm |u_n + c_c| \mp |u_n - c_c| \tag{29.2}$$

$$\gamma_n^{\pm} = u_n \pm |u_n| \tag{29.3}$$

$$\delta_n^{\pm} = -2|u_n| \pm |u_n + c_c| \pm |u_n - c_c| \tag{29.4}$$

4.3 Interpolation

We use Lagrangian elements of *nnode* nodes. Therefore, for a given time t and for a given $\boldsymbol{x} \in \Omega_{ielem}$ we interpolate the solution as:

$$\boldsymbol{U}^h(\boldsymbol{x}, t)|_{\Omega_{ielem}} = \sum_{inode=1}^{nnode} N_{ielem}^{inode}(\boldsymbol{x}) \mathcal{U}_{ielem}^{inode}(t) \tag{30}$$

where N_{ielem}^{inode} is the shape function associated to (local) node *inode* of element Ω_{ielem}.

4.4 Numerical integration

In the 2D numerical examples that we will present in this paper we have used bilinear Lagrangian elements. Numerical integration is performed by using a 3×3 points Gauss–Legendre quadrature for the elemental integrals and a three points Gauss–Legendre integration for the boundary terms.

4.5 Time integration

By assembling together all the elemental contributions, the system of ordinary differential equations that governs the evolution of the discrete solution can be written as

$$\boldsymbol{M} \frac{\mathrm{d}\mathcal{U}}{\mathrm{d}t} = \mathcal{R}(\mathcal{U}) \tag{31}$$

where $\boldsymbol{M}$ denotes the mass matrix, $\mathcal{U}$ is the global vector of degrees of freedom and $\mathcal{R}(\mathcal{U})$ is the residual vector. Due to the block diagonal structure of matrix $\boldsymbol{M}$, the time integration of this system can be accomplished in an efficient way by means of an explicit method for initial value problems. In this work we use the second order TVD-Runge–Kutta method proposed by Shu and Osher [44]. Given the solution at the nth step ($\mathcal{U}^n$), the solution at the next time level ($\mathcal{U}^{n+1}$) is computed in two steps as follows:

$$\mathcal{U}^{(1)} = \mathcal{U}^n + \Delta t \boldsymbol{L}(\mathcal{U}^n) \tag{32.1}$$

$$\mathcal{U}^{n+1} = \frac{1}{2}\mathcal{U}^n + \frac{1}{2}\mathcal{U}^{(1)} + \frac{1}{2}\Delta t \boldsymbol{L}(\mathcal{U}^{(1)}) \tag{32.2}$$

where $\boldsymbol{L}(\mathcal{U}) = \boldsymbol{M}^{-1}\mathcal{R}(\mathcal{U})$. To compute $\boldsymbol{L}(\mathcal{U})$ at each time step we do not need to calculate $\boldsymbol{M}^{-1}$. Instead of that, we compute the Cholesky factorization of the mass matrix at the first time step and we perform the necessary back and forward substitutions at each time iteration.

5 Numerical examples

In this section we solve the proposed model for mass transport in compressible fluids. The computational domain as well as the finite element mesh have been depicted in Fig. 1. The mesh has been generated by using the code GEN4U by Sarrate and Huerta [45]. The coordinates of the key points of the domain can be found in Table 1. The problem consist of a supersonic flow in a nozzle. The Mach number at the inlet takes the value $M = 1.5$ being the velocity field parallel to the walls of the nozzle at the inlet. The density and the temperature are given, respectively, by $\rho = 1.225$ kg/m^3 and $T = 288$ K. Regarding the pollutant transport, we take the value $\tau = 10^{-4}$ s for the relaxation time and $k = 0.01$ m^2/s for the diffusivity. This leads to a supercritical transport problem.

The Mach number at the steady state is plotted in Fig. 2. The maximum Mach number is $M_{\max} \approx 1.7705$. In Fig. 2 we can distinguish two rarefaction waves that are formed from points B and G. There are also shock waves generated from points C and F. We have not used any limiter to capture the shock, but we have used a fine enough mesh. The pressure at the steady state has been plotted in Fig. 3. We simulate the evolution of a pollutant being spilled at

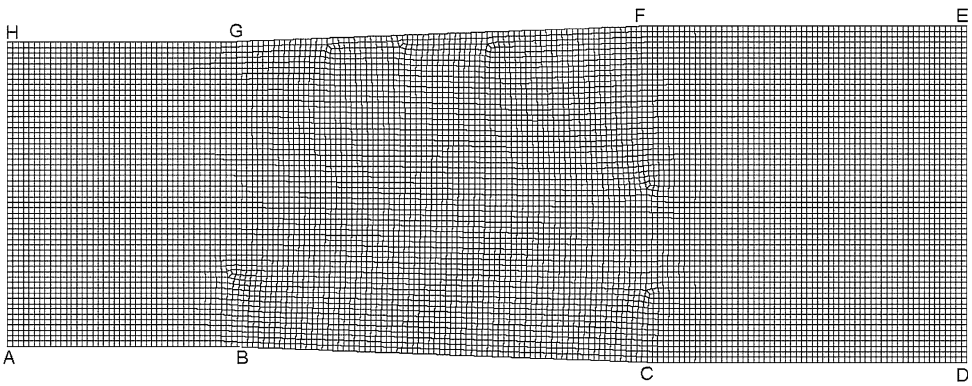

Fig. 1 Supersonic flow in a nozzle. Computational mesh (10,861 bilinear elements)

Table 1 Coordinates of the key points of the domain

Coord./Point	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*
x	0.0	20.0	60.0	90.0	90.0	60.0	20.0	0.0
y	0.0	0.0	−1.5	−1.5	30.0	30.0	28.5	28.5

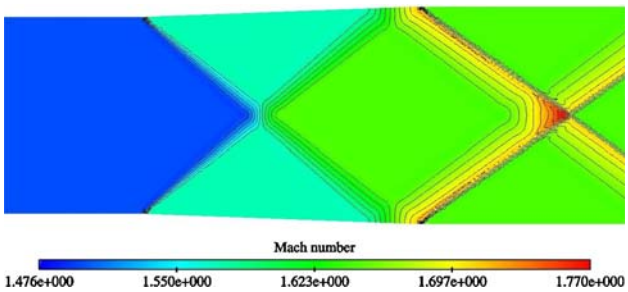

Fig. 2 Supersonic flow in a nozzle. Mach number at the steady state

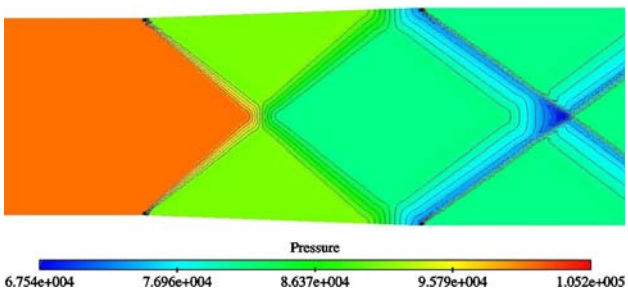

Fig. 3 Supersonic flow in a nozzle. Pressure at the steady state

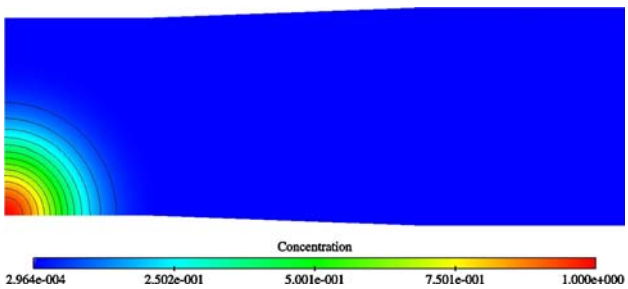

Fig. 4 Supersonic flow in a nozzle. Pollutant concentration at the initial time

the inlet of the nozzle. The initial concentration is given by $\lambda(x, y, 0) = \widehat{\lambda} e^{-0.01(x^2+y^2)}$ and it has been plotted in Fig. 4. At the initial time $\boldsymbol{q}(x,y,0) = 0$.

In Fig. 5 we represent the dimensionless concentration $\lambda/\widehat{\lambda}$ at times $t = 5 \times 10^{-2}$ s, $t = 10^{-1}$ s and at the steady state.

6 Conclusions

This paper introduces a hyperbolic model for mass transport in compressible flows. The proposed model generalizes the theory previously proposed by the authors in [24] which may be applied only to incompressible flows. A discontinuous Galerkin method is also proposed to numerically solve the governing equations. Finally, a practical example concerning engineering applications is solved to demonstrate the performance of the mathematical model and of the numerical algorithm. We conclude that the proposed model represents an interesting alternative to the standard parabolic model. However, there are some issues that should be addressed: for example those concerning the estimation of the parameters (especially the relaxation time τ) and the extension of the model to take into account non-homogeneous diffusivity and relaxation time.

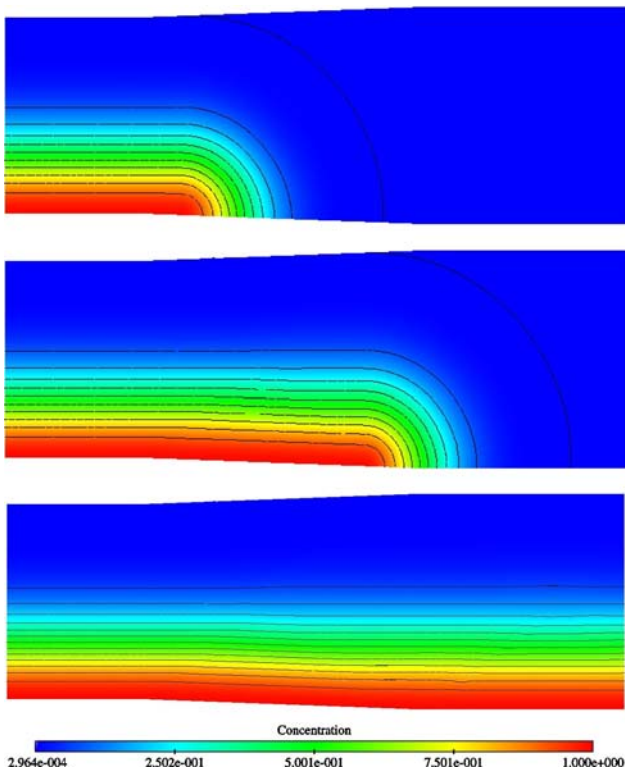

Fig. 5 Supersonic subcritical flow in a nozzle. Concentration solution at times $t = 5 \times 10^{-2}$ s, $t = 10^{-1}$ s and at the steady state

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