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A hyperbolic model for convection-diffusion transport problems in CFD: Numerical analysis and applications

H. Gómez, I. Colominas, F. Navarrina and M. Casteleiro

Abstract In this paper we present a numerical study of the hyperbolic model for convection-diffusion transport problems that has been recently proposed by the authors [16]. This model avoids the infinite speed paradox, inherent to the standard parabolic model and introduces a new parameter τ called relaxation time. This parameter plays the role of an "inertia" for the movement of the pollutant.

The analysis presented herein is twofold: first, we perform an accurate study of the 1D steady-state equations and its numerical solution. We compare the solution of the hyperbolic model with that of the parabolic model and we analyze the influence of the relaxation time on the solution. On the other hand, we explore the possibilities of the proposed model for real-world applications. With this aim we solve an example concerning the evolution of a pollutant being spilled in the harbor of A Coruña (northwest of Spain, EU).

Un modelo hiperbólico para problemas de convección-difusión en mecánica de fuidos computacional: Análisis numérico y aplicaciones

Resumen. En este artículo se presenta un estudio numérico del modelo hiperbólico para problemas de convección-difusión que ha sido recientemente propuesto por los autores [16]. Este modelo elimina la paradoja del transporte a velocidad infinita inherente al modelo parabólico e introduce un nuevo parámetro τ denominado tiempo de relajación. Este parámetro introduce una "inercia" en el movimiento del contaminante.

El artículo tiene dos objetivos: en primer lugar se realiza un detallado análisis de las ecuaciones estacionarias 1D y su solución numérica. Se compara la solución del modelo hiperbólico con la del modelo parabólico y se analiza la influencia del tiempo de relajación en la solución. El segundo objetivo es estudiar las posibilidades del modelo propuesto para aplicaciones prácticas. Para ello, se simula la evolución de un vertido contaminante en el puerto de A Coruña.

1 Introduction

There is much experimental evidence which proves that diffusive processes take place with finite velocity inside matter [6, 23]. However, standard linear parabolic models based on Fick's law [9] or Fourier's law [11] (in the case of mass transport or heat conduction respectively) predict an infinite speed of propagation. In some applications, this issue can be ignored and the use of linear parabolic models is accurate enough for practical purposes in spite of predicting an infinite speed of propagation [4]. However, in many other applications it is necessary to take into account the wave nature of diffusive processes to perform accurate predictions [6, 26].

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A great deal of effort has been devoted to the development of diffusion mathematical models that avoid the infinite speed paradox. There are two main groups which most of the models belong to: the non-linear parabolic diffusion equations and the hyperbolic diffusion equations. A detailed presentation on non-linear parabolic equations leading to finite speed of propagation can be found in the excellent book [1]. On the other hand, the hyperbolic diffusion equation was first proposed by Cattaneo [4] who introduced a generalized constitutive law[1] that includes Fick's (or Fourier's) law as a subcase. In this paper we will only study the hyperbolic theory for diffusion.

In the past, the study of hyperbolic diffusion has been limited to pure-diffusive problems [20, 21, 28, 24]. Recently the authors have proposed a generalization of the hyperbolic diffusion equation that can also be used in convective cases [12, 13, 14]. From a numerical point of view, the simulation of the hyperbolic diffusion equation has been mostly limited to 1D problems [2, 3]. The numerical discretization of 2D pure-diffusion problems was probably pioneered by Yang [27]. Later, Manzari *et al.* [22] proposed a different algorithm and solved some practical pure-diffusive examples.

The first objective of this paper is to perform an accurate analysis of the 1D steady-state convection-diffusion equation and its numerical solution. We compare the parabolic and the hyperbolic models by means of their numerical and exact solutions. The objective is to analyze whether the infinite speed paradox (inherent to the linear parabolic model) contributes or not to the non-physical oscillations that appear in convection dominated flows discretized with centered methods.

The second objective of this paper is to explore the possibilities of the hyperbolic model for practical computations in the context of mass diffusion within a fluid. In this framework, there are a number of important applications in civil and environmental engineering, for instance, the prediction of the fate of a pollutant spilled in a fluid. This paper presents an example concerning the evolution of a pollutant being spilled in the harbor of A Coruña (northwest of Spain, EU).

The outline of this paper is as follows: In Section 2 we review the parabolic formulation of the convective-diffusive equation. In section 3 we present the hyperbolic model for the transport problem. A numerical analysis of the 1D steady-state equations is performed in section 4. In section 5 we solve a practical case in environmental engineering. Finally, section 6 is devoted to the presentation of the main conclusions of this study.

2 Standard formulation of the convection-diffusion problem

2.1 Governing equations

Under the assumption of incompressibility, the governing equations are given by

$$\frac{\partial u}{\partial t} + \boldsymbol{a} \cdot \nabla_{\boldsymbol{x}}(u) + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{q}) = 0 \tag{1.1}$$

$$\boldsymbol{q} = -\boldsymbol{K} \nabla_{\boldsymbol{x}}(u) \tag{1.2}$$

In the context of mass diffusion within a fluid, (1.1) is the mass conservation equation and (1.2) is a constitutive law proposed by Fick. The notation is standard: u is the pollutant concentration, $\boldsymbol{a}$ is the velocity field, $\boldsymbol{q}$ is the diffusive flux per unit fluid density and $\boldsymbol{K}$ is the diffusivity tensor which is assumed to be positive definite.

Remark 1 *System* (1) *can be decoupled since we can plug* (1.2) *into* (1.1) *and solve the scalar equation*

$$\frac{\partial u}{\partial t} + \boldsymbol{a} \cdot \nabla_{\boldsymbol{x}}(u) - \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{K} \nabla_{\boldsymbol{x}}(u)) = 0 \tag{2}$$

[1] By constitutive law we mean a relation between two physical quantities that does not follow directly from physical law.

2.2 Problem statement

Let us consider the transport by convection and diffusion in an open set $\Omega \subset \mathbb{R}^d$ ($d = 2$ or 3) with piecewise smooth boundary Γ, such that $\Gamma = \overline{\Gamma_D \cup \Gamma_N}$. The unit outward normal vector to Γ is denoted $\boldsymbol{n}$. The convection-diffusion initial-boundary value problem can be stated as follows: given a divergence-free velocity field $\boldsymbol{a}$, the diffusion tensor $\boldsymbol{K}$ and adequate initial and boundary conditions, find $u\colon \overline{\Omega}\times[0,T] \mapsto \mathbb{R}$ such that

$$\frac{\partial u}{\partial t} + \boldsymbol{a} \cdot \nabla_{\boldsymbol{x}}(u) - \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{K}\nabla_{\boldsymbol{x}}(u)) = 0 \qquad \text{in} \quad \Omega \times (0,T) \tag{3.1}$$

$$u(\boldsymbol{x},0) = u_0(\boldsymbol{x}) \qquad \text{on} \quad \Omega \tag{3.2}$$

$$u = u_D \qquad \text{on} \quad \Gamma_D \times (0,T) \tag{3.3}$$

$$\boldsymbol{K}\nabla_{\boldsymbol{x}}(u) \cdot \boldsymbol{n} = h \qquad \text{on} \quad \Gamma_N \times (0,T) \tag{3.4}$$

3 A hyperbolic model for convection-diffusion problems

3.1 Governing equations

Under the assumption of incompressibility, the governing equations are given by

$$\frac{\partial u}{\partial t} + \boldsymbol{a} \cdot \nabla_{\boldsymbol{x}}(u) + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{q}) = 0 \tag{4.1}$$

$$\boldsymbol{q} + \boldsymbol{\tau}\left(\frac{\partial \boldsymbol{q}}{\partial t} + \nabla_{\boldsymbol{x}}(\boldsymbol{q})\,\boldsymbol{a}\right) = -\boldsymbol{K}\nabla_{\boldsymbol{x}}(u) \tag{4.2}$$

where $\boldsymbol{\tau}$ is the relaxation tensor. Equation (4.1) is the mass conservation equation and, therefore, is the same as in the parabolic model. On the contrary, equation (4.2) has been recently proposed by the authors [12, 13, 14] as a generalization of Cattaneo's law. The reason to modify Cattaneo's law comes from the fact that Cattaneo's equation was proposed for pure-diffusive problems and it does not satisfy the Galilean invariance principle. Using equation (4.2) the description of the diffusion process is granted to be the same in every inertial frame [5]. Additionally, when the domain is fixed ($\boldsymbol{a} = 0$) the original Cattaneo's law is recovered.

Remark 2 *System (4) constitutes a generalization of the classic parabolic convection-diffusion model since the standard formulation is recovered by setting* $\boldsymbol{\tau} = 0$.

Remark 3 *System (4) can be written as a single second order partial differential equation when the velocity field is constant [12].*

Remark 4 *The proposed model may also be combined with non-linear diffusivities (dependent on the solution or its derivatives). The authors believe this could lead to an interesting convection-diffusion model and they are currently studying that model.*

3.2 Conservative form of the proposed equations

Under the hypotheses of isotropy and homogeneity $\boldsymbol{K} = k\boldsymbol{I}$, $\boldsymbol{\tau} = \tau\boldsymbol{I}$ for certain $k, \tau \in \mathbb{R}^+$, being $\boldsymbol{I}$ the identity tensor. This allows for a conservative form of system (4), namely

$$\frac{\partial u}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (u\boldsymbol{a} + \boldsymbol{q}) = 0 \tag{5.1}$$

$$\frac{\partial (\tau\boldsymbol{q})}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\tau\boldsymbol{q} \otimes \boldsymbol{a} + ku\boldsymbol{I}) + \boldsymbol{q} = 0 \tag{5.2}$$

Also, defining the vectors

$$\boldsymbol{U} = \left(\frac{u}{\tau \boldsymbol{q}} \right); \quad \boldsymbol{F} = \left(\frac{(u\boldsymbol{a} + \boldsymbol{q})^T}{\tau \boldsymbol{q} \otimes \boldsymbol{a} + ku\boldsymbol{I}} \right); \quad \boldsymbol{S} = \left(\frac{0}{-\boldsymbol{q}} \right) \tag{6}$$

system (5) can be rewritten in the standard conservative form

$$\frac{\partial \boldsymbol{U}}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{F}) = \boldsymbol{S} \tag{7}$$

An standard Riemann analysis of equation (7) yields the following conclusions (see [15] for the details)

1. System (7) is totally hyperbolic for any admisible value of the parameters of the model k and τ
2. It is possible to define the so-called Riemann quasi-invariants for a given direction. We will call $\boldsymbol{R_n}$ the Riemann quasi-invariants at the boundary in the direction of $\boldsymbol{n}$, the outward normal to the boundary. Also, we will denote $\boldsymbol{R_n^{\text{in}}}$ (where the superscript in stands for inflow) the $\boldsymbol{R_n}$ quasi-invariants that corresponds to negative eigenvalues.
3. The dimensionless number
$$H = \frac{\|\boldsymbol{a}\|}{c} \tag{8}$$
allows for the flow to be classified as
    - $H < 1 \Leftrightarrow$ Subcritical flow.
    - $H > 1 \Leftrightarrow$ Supercritical flow.
    - $H = 1 \Leftrightarrow$ Critical flow.
4. Appropriate boundary conditions to define a well-posed initial-boundary problem from system (7) are obtained precribing at each point of the boundary the value of $\boldsymbol{R_n^{\text{in}}}$

Remark 5 *The dimensionless number H defined in (8) plays a similar role to Mach number in compressible flow problems [7]. We remark that in supercritical flow the pollutant cannot travel upstream, since its velocity is smaller than the fluid velocity.*

4 Numerical analysis of the 1D steady-state equations: the connection between the parabolic and the hyperbolic model

4.1 The antidiffusion introduced by Cattaneo's law

In this section we show that, under adequate assumptions, Cattaneo's law introduces a negative diffusion with respect to Fick's law. We make use of the governing equations for the steady-state, namely

$$\nabla_{\boldsymbol{x}} \cdot (\boldsymbol{F}) = \boldsymbol{S} \tag{9}$$

The above equation can be rewritten as

$$\frac{\mathrm{d}q}{\mathrm{d}x} = -a\frac{\mathrm{d}u}{\mathrm{d}x} \tag{10.1}$$

$$k\frac{\mathrm{d}u}{\mathrm{d}x} + \tau a\frac{\mathrm{d}q}{\mathrm{d}x} = -q \tag{10.2}$$

If we use (10.1) and the derivative of (10.2), the following second order equation is found:

$$a\frac{\mathrm{d}u}{\mathrm{d}x} - (k - \tau a^2)\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} = 0 \tag{11}$$

Equation (11) shows clearly that Cattaneo's law introduces a negative diffusion with respect to Fick's law. It may be argued that this fact represents an important drawback of the hyperbolic model because it complicates the numerical resolution of the equation. This is not true. A discussion on this point will be presented in section 4.4.

Remark 6 *Equation (11) can be only thought of as the standard parabolic model with a negative diffusion in subcritical flow. In this case the term $k - \tau a^2$ remains positive. In supercritical flow equation (11) still makes sense, but the term $k - \tau a^2$ cannot be thought of as a diffusivity.*

Remark 7 *Equation (11) is not equivalent to system (9). The hyperbolic model for convection-diffusion is given by system (9) and not by equation (11). However, in the case of subcritical flow and Dirichlet boundary conditions both formulations are equivalent if the solutions are sufficiently smooth.*

4.2 The effect of the standard Galerkin discretization on the classic parabolic convection-diffusion equation

We analyze the classic parabolic convection-diffusion problem subject to Dirichlet boundary conditions. We use the following model problem: find $u\colon [0,L] \mapsto \mathbb{R}$ such that

$$a\frac{\mathrm{d}u}{\mathrm{d}x} - k\frac{\mathrm{d}^2u}{\mathrm{d}x^2} = 0; \quad x \in (0,L) \tag{12.1}$$

$$u(0) = u_0 \tag{12.2}$$

$$u(L) = u_L \tag{12.3}$$

Let $\mathcal{P}$ be a uniform partition of $[0,L]$ defined by the points $\{x_i\}_{i=0,N}$ such that $x_i = (i-1)h$, being $h = L/(N-1)$. Let us call

$$P_{\mathsf{e}} = \frac{ah}{2k} \tag{13}$$

the *mesh Péclet number* which expresses the ratio of convective to diffusive transport. If we solve (12) by using the standard Galerkin method and linear finite elements (this is equivalent to second-order centered finite differences for this case) we obtain the following discrete equation at an interior node j:

$$(1 - P_{\mathsf{e}})u_{j+1} - 2u_j + (1 + P_{\mathsf{e}})u_{j-1} = 0 \tag{14}$$

In equation (14) u_j is the finite element approximation of $u(x_j)$ and u_0, u_N are the values given by boundary conditions (12.2)–(12.3). Difference equations (14) can be solved exactly (see, for instance, reference [19]). The exact solution of (14), subject to boundary conditions (12.2)–(12.3), is

$$u_j = \frac{1}{1 - \left(\frac{1+P_{\mathsf{e}}}{1-P_{\mathsf{e}}}\right)^N} \left\{ u_0 \left[\left(\frac{1+P_{\mathsf{e}}}{1-P_{\mathsf{e}}}\right)^j - \left(\frac{1+P_{\mathsf{e}}}{1-P_{\mathsf{e}}}\right)^N \right] + u_L \left[1 - \left(\frac{1+P_{\mathsf{e}}}{1-P_{\mathsf{e}}}\right)^j \right] \right\} \tag{15}$$

From equation (15) it is observed that the numerical solution will present an oscillatory behavior[2] when $|P_{\mathsf{e}}| > 1$, even though equations (14) were solved exactly. On the other hand, the exact solution of (12) is

$$u(x_j) = \frac{1}{1 - e^{\frac{ah}{k}N}} \left[u_0 \left(e^{\frac{ah}{k}j} - e^{\frac{ah}{k}N} \right) + u_L \left(1 - e^{\frac{ah}{k}j} \right) \right] \tag{16}$$

[2]These non-physical oscillations are normally referred to as *wiggles* or *node-to-node oscillations* in the Computational Mechanics community. A numerical solution that presents this behavior is normally said to be *unstable*. Although we are aware that this is not an stability issue since we are considering the exact solution of the discrete equations (14), we will use this nomenclature in the rest of the paper.

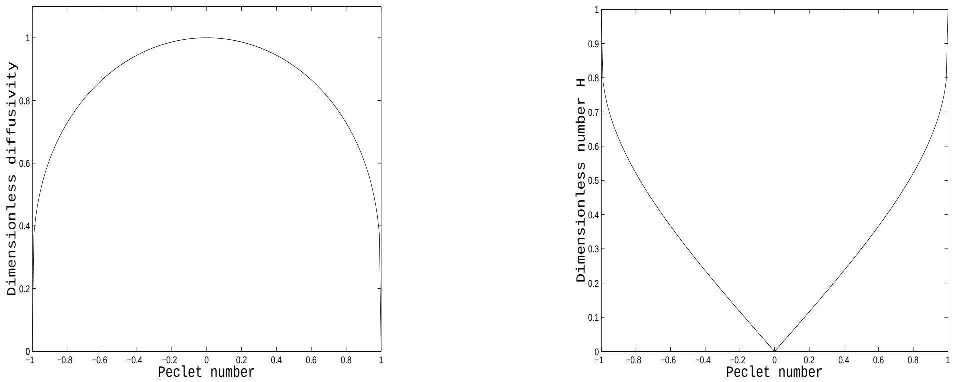

Figure 1. Dimensionless diffusivity ($k^\star/k$) as a function of P_e (left) and dimensionless number H as a function of P_e (right).

A comparison between (15) and (16) shows that the approximate solution equals the exact solution if the following relation holds

$$e^{2P_\mathrm{e}j} = \left(\frac{1+P_\mathrm{e}}{1-P_\mathrm{e}}\right)^j \quad \forall j = 0, N \tag{17}$$

Relation (17) is only satisfied for $P_\mathrm{e} = 0$ (pure-diffusive problem). However, using (17) we find that when the mesh is fine enough ($|P_\mathrm{e}| \leq 1$) the approximate solution (15) is, actually, the exact solution of the problem

$$a\frac{\mathrm{d}u}{\mathrm{d}x} - k^\star\frac{\mathrm{d}^2u}{\mathrm{d}x^2} = 0; \quad x \in (0, L) \tag{18.1}$$

$$u(0) = u_0 \tag{18.2}$$

$$u(L) = u_L \tag{18.3}$$

where

$$k^\star = k\frac{2P_\mathrm{e}}{\ln\left(\frac{1+P_\mathrm{e}}{1-P_\mathrm{e}}\right)} \tag{19}$$

On the left hand side of figure 1 we represent $k^\star/k$ as a function of $P_\mathrm{e} \in (-1, 1)$. We observe that $k^\star \to k$ as $|P_\mathrm{e}| \to 0$ and $k^\star \to 0$ as $|P_\mathrm{e}| \to 1$.

Remark 8 *If the mesh is fine enough ($|P_\mathrm{e}| < 1$), then $k^\star \in (0, k]$, what means that the standard Galerkin method solves exactly an underdiffusive equation. If the mesh is not fine enough ($|P_\mathrm{e}| > 1$), then $k^\star$ becomes complex and it is not correct anymore to say that the standard Galerkin method solves an underdiffusive equation.*

Remark 9 *Equation (12.1) can be thought of as Newton's equation for a particle under viscous damping when $a < 0$. In this case, the element Peclet number P_e is proportional to the variation of the kinetic energy of the particle in the discrete sense, which suggests that the Peclet number is related to stability.*

4.3 The connection between the hyperbolic model and the discretized parabolic model

We prove that (under the necessary assumptions) when a standard Galerkin discretization is applied to the classic parabolic convection-diffusion equation, the velocity of propagation is not infinite anymore at the discrete level. On the contrary, a finite velocity of propagation can be identified in the discrete equations. We conclude that the standard Galerkin formulation introduces an "artificial" relaxation time. The proof requires $k^\star$ to be rearranged as

$$k^\star = k - k\left(1 - \frac{2P_\mathsf{e}}{\ln\left(\frac{1+P_\mathsf{e}}{1-P_\mathsf{e}}\right)}\right) < k \tag{20}$$

If we compare the diffusive coefficient $k^\star$ with the coefficient which results from using Cattaneo's law (this can be found in equation (11)) the following conclusion is achieved: when we solve (12) by using the standard Galerkin method we obtain the solution of a Cattaneo-type transport problem defined by the relaxation time

$$\tau_G = \frac{h}{a}\left(\frac{1}{2P_\mathsf{e}} - \frac{1}{\ln\left(\frac{1+P_\mathsf{e}}{1-P_\mathsf{e}}\right)}\right) \tag{21}$$

As a result, a finite velocity of propagation can be defined in the discrete equation (14), namely

$$c_G = \frac{a}{\left(1 - \frac{2P_\mathsf{e}}{\ln\left(\frac{1+P_\mathsf{e}}{1-P_\mathsf{e}}\right)}\right)^{1/2}} \tag{22}$$

By using the relation (22) it is easy to compute the value of "artificial" H (see equation (8) for a definition of H) introduced by the Galerkin method for a certain P_e. In figure 1 (right) we plot the "artificial" H as a function of P_e.

We conclude that when we solve problem (12) for $|P_\mathsf{e}| < 1$ by using the standard Galerkin method we are actually solving a Cattaneo-type transport problem in subcritical flow conditions. To summarize, we present the relationships between the hyperbolic and the parabolic model at the continuous and discrete level in figure 2.

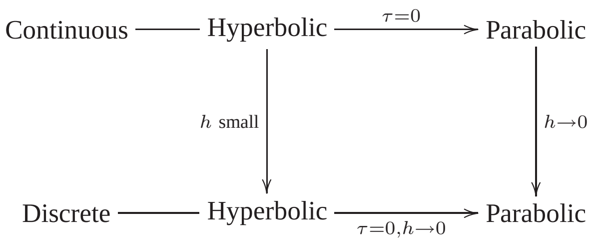

Figure 2. Relationship between the parabolic and the hyperbolic model at the continuous and discrete level.

Remark 10 *The Cattaneo-type problem that is being actually solved is given by*

$$a\frac{\mathrm{d}u}{\mathrm{d}x} - (k - \tau_G a^2)\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} = 0; \quad x \in (0, L) \tag{23.1}$$

$$u(0) = u_0 \tag{23.2}$$

$$u(L) = u_L \tag{23.3}$$

where τ_G is defined in equation (21). Problem (23) is a well-posed boundary-value problem for every value of the parameters k and τ_G. However, it only represents a Cattaneo-type convection-diffusion problem in *subcritical flow. As we said before, equation (23.1) can be (under the assumption of sufficient regularity) used to describe the steady-state hyperbolic model, but boundary conditions have to be set in such a way that (7) is well-posed. Since (7) is not well-posed subject to boundary conditions (23.2)–(23.3) in supercritical flow, problem (23) does not represent anymore a Cattaneo-type convection-diffusion problem in supercritical flow.*

4.4 Stability analysis of the hyperbolic model

Let us consider again the partition $\mathcal{P}$ that defines the mesh size h. We introduce the dimensionless number

$$H_{\mathsf{e}} = \frac{ah}{2(k - \tau a^2)} \tag{24}$$

which plays a similar role to P_{e} in the standard description of the transport problem [13, 14]. If we solve (23) by using the standard Galerkin method and linear finite elements (this is equivalent to second-order centered finite differences for this case), the following difference equations are found [12]:

$$(1 - H_{\mathsf{e}})u_{j+1} - 2u_j + (1 + H_{\mathsf{e}})u_{j-1} = 0; \quad \forall j = 1, \ldots, N-1 \tag{25}$$

In the same way as (14), difference equations (25) can be solved exactly and the stability condition

$$|H_{\mathsf{e}}| \leq 1 \tag{26}$$

can be found. Relation (26) suggests that in the hyperbolic model numerical instabilities do not arise for large values of the fluid velocity a, but they appear for values of $|a|$ close to the pollutant velocity c. Indeed, the size (in the velocity domain) of the interval that leads to unstable solutions is

$$I = h/\tau \tag{27}$$

we prove the above assertion by finding the a values that make

$$|H_{\mathsf{e}}| = 1 \tag{28}$$

which are given by

$$a_1 = -\frac{h}{4\tau} - \sqrt{\left(\frac{h}{4\tau}\right)^2 + c^2} \tag{29.1}$$

$$a_2 = -\frac{h}{4\tau} + \sqrt{\left(\frac{h}{4\tau}\right)^2 + c^2} \tag{29.2}$$

$$a_3 = -a_2 \tag{29.3}$$

$$a_4 = -a_1 \tag{29.4}$$

It is straightforward that $a_1 < 0$, $a_1 < -c$, $a_2 > 0$, $a_2 < c$. Taking into account all of this, the interval of velocities that makes the numerical solution unstable has a size of

$$I = a_4 - a_2 + a_3 - a_1 = -2(a_1 + a_2) = h/\tau \tag{30}$$

as we said above.

Remark 11 *The size of the interval I decreases as τ increases which suggests that the transport problem becomes more stable as τ increases.*

Remark 12 *All the theoretical results presented in section 4 have been confirmed by numerical experiments in [15].*

Figure 3. Simulation of an accidental spillage in the port of A Coruña. Digital photograph showing the port.

5 An application example: simulation of an accidental spillage in the port of A Coruña

The objective of this section is to investigate the possibilities of the proposed hyperbolic system as a model for real-world applications. We are interested in practical applications in civil and environmental engineering. For this reason, we present an example concerning the evolution of an accidental spillage in the harbor of A Coruña (northwest of Spain, EU).

5.1 Numerical algorithm

5.1.1 Continuous problem in the weak form

We begin by considering a weak form of the hyperbolic convection-diffusion model. Let $\mathcal{V}$ denote the trial solution and weighting functions spaces, which are assumed to be the same. Therefore, the variational formulation is stated as follows: find $\boldsymbol{U} \in \mathcal{V}$ (we assume that this implies strong satisfaction of boundary conditions) such that $\forall \boldsymbol{W} \in \mathcal{V}$,

$$B_C(\boldsymbol{W}, \boldsymbol{U}) = 0 \tag{31}$$

where

$$B_C(\boldsymbol{W}, \boldsymbol{U}) = \left(\boldsymbol{W}, \frac{\partial \boldsymbol{U}}{\partial t}\right)_\Omega - (\nabla_{\boldsymbol{x}}(\boldsymbol{W}), \boldsymbol{F})_\Omega + (\boldsymbol{W}, \boldsymbol{F}\boldsymbol{n})_\Gamma - (\boldsymbol{W}, \boldsymbol{S})_\Omega \tag{32}$$

being $(\cdot\,,\cdot)_\Omega$ the L^2-inner product with respect to the domain Ω. The integration by parts of equation of (32), under the assumption of sufficient regularity, leads to the Euler-Lagrange form of (32)

$$\left(\boldsymbol{W}, \frac{\partial \boldsymbol{U}}{\partial t}\right)_\Omega + (\boldsymbol{W}, \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{F}))_\Omega - (\boldsymbol{W}, \boldsymbol{S})_\Omega = 0 \tag{33}$$

which implies the weak satisfaction of equation (7)

5.1.2 Time integration

For the time integration we replace the time derivative in (32) by its second order Taylor expansion, namely

$$\frac{\partial \boldsymbol{U}}{\partial t}(\cdot, t^n) = \frac{\boldsymbol{U}(\cdot, t^{n+1}) - \boldsymbol{U}(\cdot, t^n)}{\Delta t} - \frac{\Delta t}{2}\frac{\partial^2 \boldsymbol{U}}{\partial t^2}(\cdot, t^n) + \theta(\Delta t^2) \tag{34}$$

where $\Delta t = t^{n+1} - t^n$ and $\theta(\Delta t^2)$ is an error of the order of Δt^2. Using the notation $\Delta t \Delta \boldsymbol{U}(\cdot) = \boldsymbol{U}(\cdot, t^{n+1}) - \boldsymbol{U}(\cdot, t^n)$ and rewritting the second-order time derivative in (34) in terms of spatial derivatives using the original equation (7), the following variational equation is found (see the details in [15]): find $\boldsymbol{U} \in \mathcal{V}$ such that $\forall \boldsymbol{W} \in \mathcal{V}$

$$B_{SD}(\boldsymbol{W}, \boldsymbol{U}) = 0 \tag{35}$$

being

$$\begin{aligned} B_{SD}(\boldsymbol{W}, \boldsymbol{U}) = (\boldsymbol{W}, \Delta \boldsymbol{U})_\Omega &- \left(\boldsymbol{W}, \Delta t \boldsymbol{B}(\boldsymbol{I} + \frac{\Delta t}{2}\boldsymbol{B})\boldsymbol{U}\right)_\Omega \\ &- \left(\frac{\partial \boldsymbol{W}}{\partial x_i}, \Delta t(\boldsymbol{I} + \Delta t \boldsymbol{B})\boldsymbol{A}_i \boldsymbol{U} - \frac{\Delta t^2}{2}\boldsymbol{A}_i \boldsymbol{A}_j \frac{\partial \boldsymbol{U}}{\partial x_j}\right)_\Omega \\ &+ \left(\boldsymbol{W}, \Delta t(\boldsymbol{I} + \Delta t \boldsymbol{B})\boldsymbol{A}_i n_i \boldsymbol{U} - \frac{\Delta t^2}{2} n_i \boldsymbol{A}_i \boldsymbol{A}_j \frac{\partial \boldsymbol{U}}{\partial x_j}\right)_\Gamma \end{aligned} \tag{36}$$

where the $\boldsymbol{A}_i$'s are the Jacobian matrices of the flux $\boldsymbol{F}$, the n_i's are the components of $\boldsymbol{n}$, $\boldsymbol{B}$ is the Jacobian matrix of the source term $\boldsymbol{S}$ and the Einstein summation convection has been used.

5.1.3 Space discretization

For the space discretization of (36) we make use of the Galerkin method. We approximate (35)–(36) by the following variational problem over the finite element spaces: find $\boldsymbol{U} \in \mathcal{V}^h$ such that $\forall \boldsymbol{W} \in \mathcal{V}^h$

$$B_{SD}(\boldsymbol{W}^h, \boldsymbol{U}^h) = 0 \tag{37}$$

For equation (37) to be well defined our discrete spaces have to be $\mathcal{H}^1$-conforming. We will use $\mathcal{C}^0$-continuous linear finite elements which satisfy this requirement.

Remark 13 *The presented algorithm is based on the second-order Taylor-Galerkin method that was first proposed in* [8].

5.2 Problem setup

The domain of the problem comprises the whole area of the A Coruña port. In figure 3 we show a digital photograph of the port. We represent the layout of the port in figure 4. To bound the domain of the problem we define an open-sea boundary from the end of Barrie's dike to the extreme of Oza's dock. The resulting computational domain has been depicted in figure 5 (left). As it can be seen in this figure some elements of the real domain have been removed in order to simplify the generation of the mesh. However, the omission of these elements is not important for the solution of the problem [10]. For instance, the oil tanker pier allows both water and pollutant to flow through it, so it does not modify the solution.

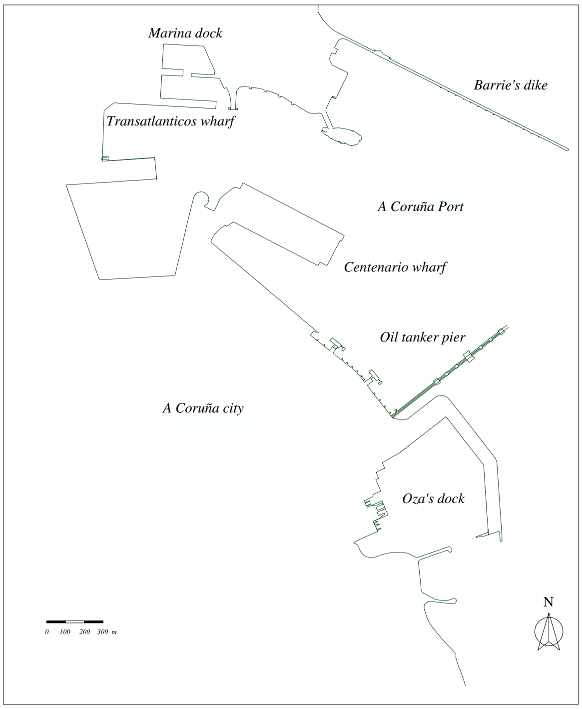

Figure 4. Simulation of an accidental spillage in the port of A Coruña. Layout of the port.

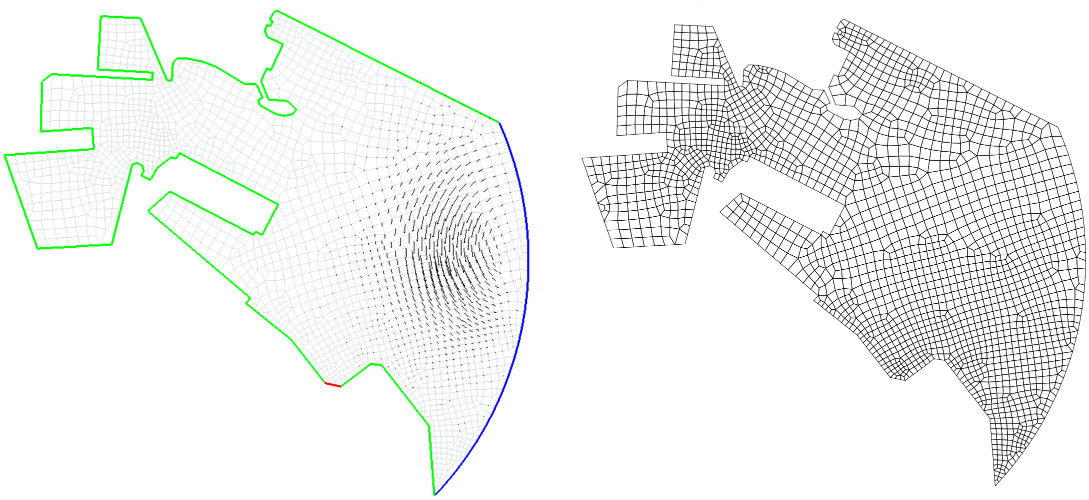

Figure 5. Simulation of an accidental spillage in the port of A Coruña. Velocity field and kinds of boundaries (left) and computational mesh of the problem (right). On the left hand side the solid wall boundary has been plotted in green; the boundary where the spillage happens has been plotted in red; the open sea boundary has been plotted in blue. The finite element mesh consists of 2023 bilinear elements and it was generated by using the code GEN4U [25].

Three kinds of boundaries are differentiated in figure 5 (left): the solid wall boundary has been plotted in green; the boundary where the spillage happens has been plotted in red; the open-sea boundary has been plotted in blue.

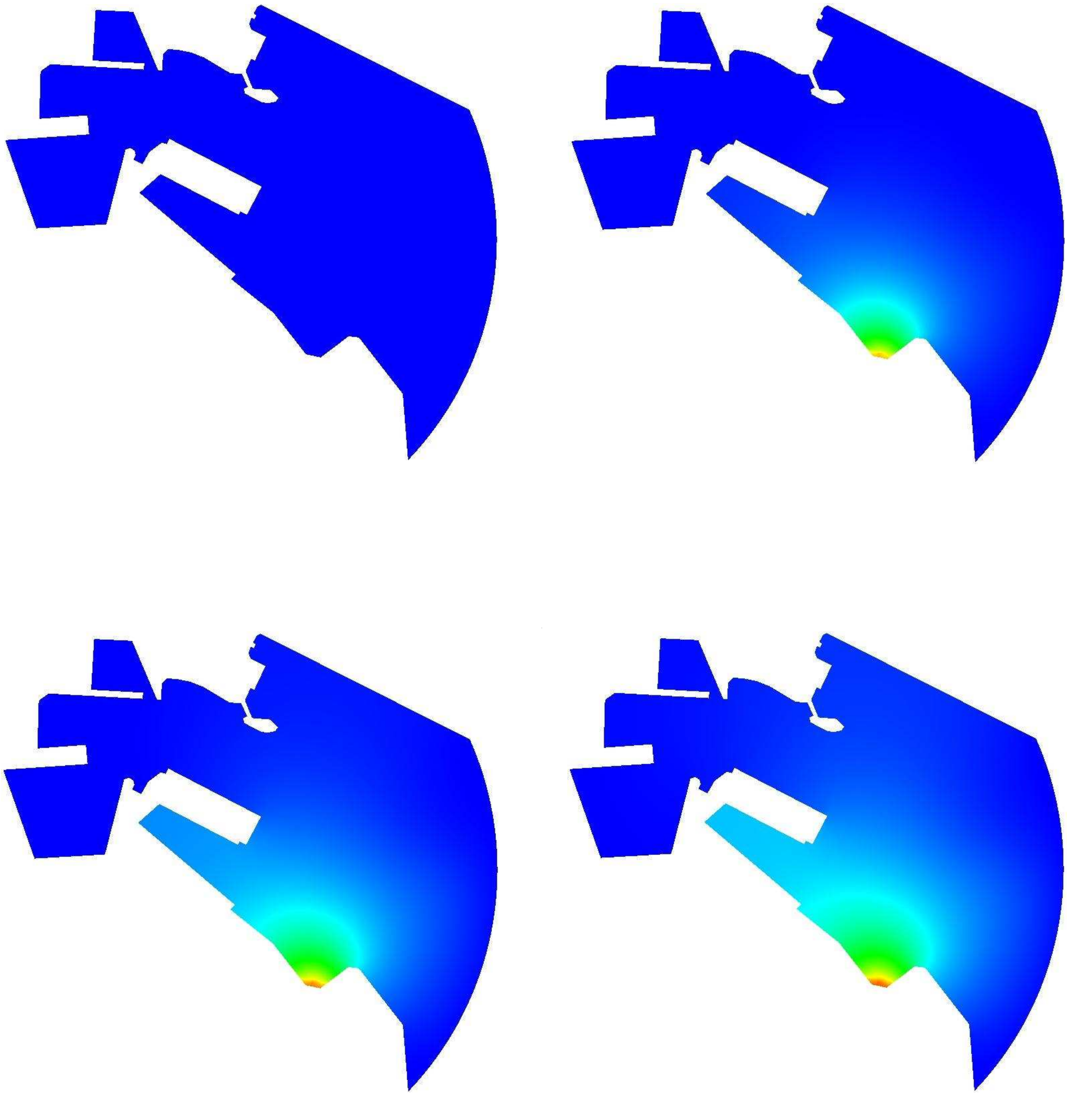

Figure 6. Simulation of an accidental spillage in the port of A Coruña. We show (left to right and top to bottom) the concentration initial condition and concentration solutions at non-dimensional times $t^* = 30$, $t^* = 60$ and $t^* = 90$.

The objective of this example is to show that the proposed methodology can be used to simulate real-world problems. For this reason we have not considered necessary to perform an accurate estimation of the parameters which would entail a lot of experimental work. A typical value for engineering calculations has been selected for the diffusivity k [18]. The estimation of the relaxation time τ is not so trivial since only the order of magnitude of the parameter can be estimated without making experiments. However, what really determines the solution is the velocity of the fluid $\boldsymbol{a}$ with respect to the velocity of the pollutant $c = \sqrt{k/\tau}$.

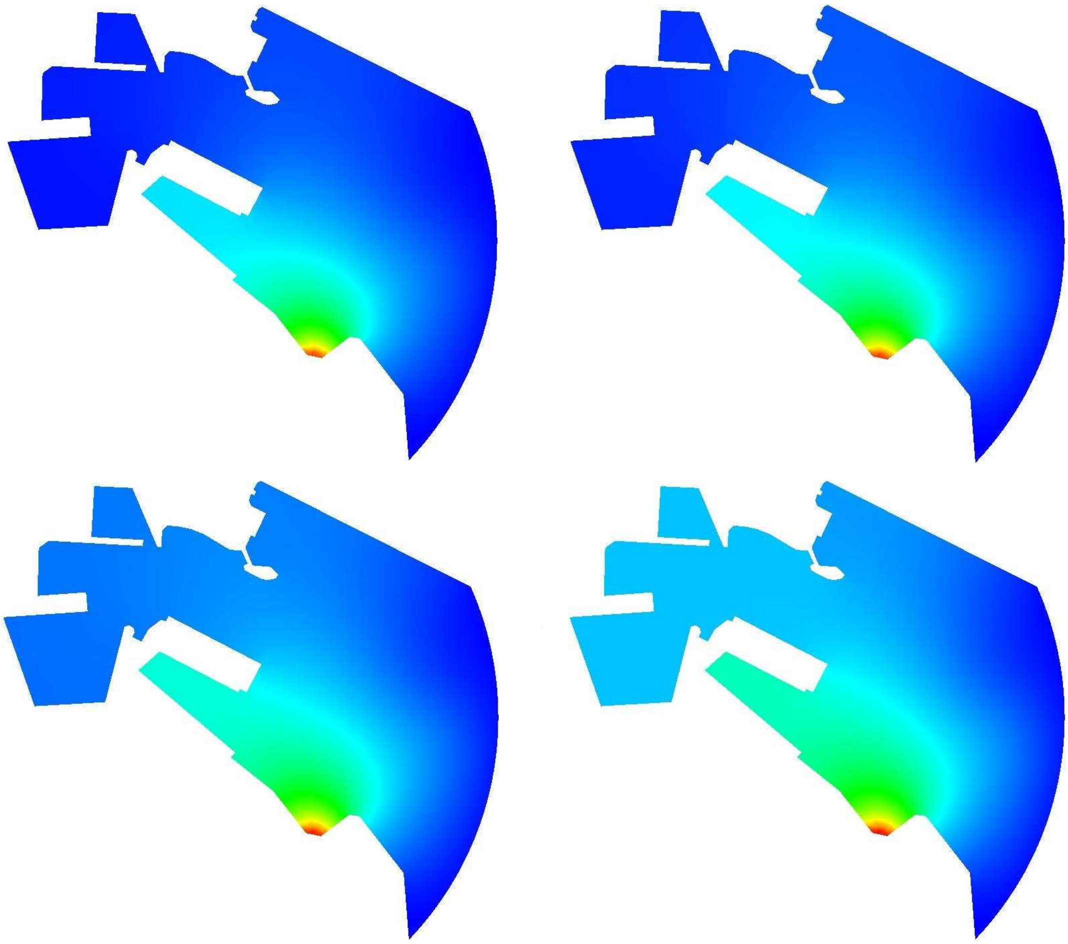

Figure 7. Simulation of an accidental spillage in the port of A Coruña. We show (left to right and top to bottom) concentration solutions at non-dimensional times $t^* = 120$, $t^* = 150$, $t^* = 300$ and $t^* = 1000$.

This quotient defines a Mach-type number as it can be seen in equation (8).

In order to reduce the computations, the velocity field has not been calculated, but it was generated with two constraints: a) it verifies the continuity equation for incompressible flow and b) it satisfies standard boundary conditions for a viscous flow. The velocity field has been plotted in figure 5 (left). On the right hand side of figure 5 we have depicted the computational mesh.

On the solid wall boundary we impose $\boldsymbol{q} \cdot \boldsymbol{n} = 0$. On the boundary where the spillage takes place the condition $\boldsymbol{q} \cdot \boldsymbol{n} = -10^{-2}$ is imposed. On the open-sea boundary we impose $\boldsymbol{q} \cdot \boldsymbol{n} = cu$ where $c = \sqrt{k/\tau}$ is the pollutant wave velocity. The flow is given by H numbers ($H = \|\boldsymbol{a}\|/c$) verifying $H \leq H_{\max} \approx 0.3237$ what makes the problem to be subcritical at each point of the domain. The computation was performed taking a maximum CFL number $C_{\max} \approx 0.5531$.

At this point we define the non-dimensional time $t^* = t/\tau$. In figure 6 we show the initial concentration and concentration solutions at non-dimensional times $t^* = 30$, $t^* = 60$ and $t^* = 90$. In figure 7 concentration solutions at non-dimensional times $t^* = 120$, $t^* = 150$, $t^* = 300$ and $t^* = 1000$ are plotted.

Remark 14 *This computation was repeated on finer meshes in space and time. Also, the calculations were repeated using a Runge-Kutta discontinuous Galerkin method* [17]*. No significant differences were found in any case.*

6 Conclusions and future developments

In this paper, a hyperbolic model for convection-diffusion problems in CFD is analyzed. The hyperbolic formulation avoids the infinite speed paradox inherent to the standard linear parabolic formulation. The proposed formulation constitutes a generalized approach for convective-diffusive phenomena because the standard formulation can be considered as a subcase of the proposed one.

From a numerical point of view, we have shown that the discrete equations of the Fick-type 1D steady model represent, actually, a Cattaneo-type transport problem when the standard Galerkin formulation is employed. In addition, we show that the Galerkin solution (with linear finite elements) of the proposed equations is stable for any value of the fluid velocity except for a small interval which length decreases as the relaxation time increases.

Finally, we present an application in environmental engineering in order to explore the possibilities of the hyperbolic model for real computations. We conclude that the proposed model is a feasible alternative to the standard parabolic models. However, there are some issues that should be addressed: for example those concerning the computational cost of the numerical approach and the estimation of the parameters of the model (especially the relaxation time τ).

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H. Gómez
Institute for Comp. Eng. and Sciences
University of Texas at Austin
201 East 24th Street, ACES 5.428
Austin, TX 78712-0027
and
Departamento de Métodos Matemáticos
Universidad de A Coruña
Campus de Elviña, s/n
15192 A Coruña

I. Colominas
Departamento de Métodos Matemáticos
Universidad de A Coruña
Campus de Elviña, s/n
15192 A Coruña

F. Navarrina
Departamento de Métodos Matemáticos
Universidad de A Coruña
Campus de Elviña, s/n
15192 A Coruña

M. Casteleiro
Departamento de Métodos Matemáticos
Universidad de A Coruña
Campus de Elviña, s/n
15192 A Coruña