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L^∞ -stability of IMEX-BDF2 finite volume scheme for convection-diffusion equation

Caterina Calgaro and Meriem Ezzoug

Abstract In this paper, we propose a finite volume scheme for solving a two-dimensional convection-diffusion equation on general meshes. This work is based on a implicit-explicit (IMEX) second order method and it is issued from the seminal paper [2]. In the framework of MUSCL methods, we will prove that the local maximum property is guaranteed under an explicit Courant-Friedrichs-Levy condition and the classical hypothesis for the triangulation of the domain.

Key words: Convection-diffusion equation, finite volume scheme, IMEX-BDF2 scheme, L^∞ -stability

MSC (2010): 65M99, 76M12, 76E17

1 Introduction

Convection-diffusion processes appear in many areas of science, e.g. fluid dynamics or heat and mass transfer. In the study of the evolution of a mixture, the system of PDEs derives from the compressible Navier-Stokes equations. The mixture of two viscous fluids is described by the density $\rho \geq 0$, the *mass velocity* field \mathbf{v} (which is not solenoidal) and the pressure p . Following Kazhikhov and Smagulov [11], we set

$$\mathbf{u} = \mathbf{v} + \lambda \nabla \ln(\rho), \quad (1)$$

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for some mass diffusion coefficient $\lambda > 0$. This Fick's law describes the diffusive fluxes of one fluid into the other. Clearly, the *volume velocity* field \mathbf{u} satisfies $\operatorname{div} \mathbf{u} = 0$ and we obtain the non-standard constraint $\operatorname{div} \mathbf{v} = -\operatorname{div}(\lambda \nabla \ln(\rho))$, which is relied on the definition of the pressure p . Using (1), the mass conservation equation becomes

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{u}) = \lambda \Delta \rho. \quad (2)$$

The momentum equation can also be rewritten in order to obtain the Kazhikhov-Smagulov model [11]. This model was firstly studied in [14, 1] (see also references therein). The mathematical analysis in a three-dimensional domain of Kazhikhov-Smagulov type models was carried out in recent works [5, 8], where the authors study the Kazhikhov-Smagulov models with a specific Korteweg stress tensor. The numerical study of a Kazhikhov-Smagulov model for the two-dimensional case can be found in [4], where the authors propose an hybrid finite volume-finite element method combined with the backward Euler method in time. In order to generalize the analysis given in [4] to second-order methods in time and space, the first goal is to recover the L^∞ -stability of the finite volume method used for the convection-diffusion equation. This is the purpose of this paper.

2 Description of the numerical scheme

This section is devoted to the design of a numerical scheme to approximate (2), using the vertex-based MUSCL finite volume methods introduced in [13] and used in [2] for a second-order accuracy in space, and an implicit-explicit (IMEX) linear multistep methods [10] for a second-order in time.

Mesh definitions and notations. Let Ω be an open bounded polygonal subset on \mathbb{R}^2 , with sufficiently regular boundary $\partial\Omega$, and $[0, T]$ the time interval, for $T > 0$. The discretization of (2) will be carried out on an unstructured triangular mesh. We denote by \mathcal{T}_h a partition of Ω composed of conforming and isotropic triangles T_k , $k \in [1, K]$, with $K \in \mathbb{N}^*$. The \mathcal{T}_h is called the *primal mesh*. We suppose the following hypotheses:

- (H1) Let $\{\mathcal{T}_h\}_{h>0}$ be a *regular* family of triangulations of Ω .
- (H2) The triangulation \mathcal{T}_h is of *weakly acute type* (no triangle with an angle greater than $\pi/2$).

For each element $T \in \mathcal{T}_h$, we denote B_T the barycenter of the triangle, $|T|$ the area of T , and M_i, M_{j_1}, M_{j_2} the three vertices of T . We also denote respectively $M_{i_{j_1}}$ and $M_{i_{j_2}}$ the middles of $[M_i M_{j_1}]$ and $[M_i M_{j_2}]$.

Let us construct the *dual mesh* $\mathcal{C}_h = \{\mathcal{C}_i, i \in [1, I]\}$, which defines a second partition of Ω , ($I \in \mathbb{N}^*$ is the number of vertices of \mathcal{T}_h). The dual finite volume \mathcal{C}_i associated with each vertex M_i , $i \in [1, I]$, is a closed polygon obtained in the following way: we join the barycenter B_T of every triangle $T \in \mathcal{T}_h$ which share the vertex M_i with

the middle point of every side of T containing M_i (see Fig. 1). If $M_i \in \partial\Omega$, then we complete the boundary of \mathcal{C}_i by the segments joining M_i with the middle point of boundary sides that contain M_i . \mathcal{C}_i is often called the vertex-based control volume around the node M_i . Accordingly, we have $\cup_{T \in \mathcal{T}_h} T = \bar{\Omega} = \cup_{i \in [1, I]} \mathcal{C}_i$.

Moreover, if we denote $|\mathcal{C}_i|$ the area of $\mathcal{C}_i \in \mathcal{C}_h$, then $|\mathcal{C}_i| = \sum_{T, M_i \in T} \frac{|T|}{3}$.

For $i \in [1, I]$, let $\mathcal{V}(i) = \{j \in [1, I], \mathcal{C}_j \text{ is a neighbor of } \mathcal{C}_i\}$. For $l = 1, 2$, we denote $\Gamma_{ij_l}^{(T)}$ the segment $[M_{ij_l} B_T]$, $A_{ij_l}^{(T)}$ its middle point, $\mathbf{n}_{ij_l}^{(T)}$ the unit outward normal to \mathcal{C}_i along $\Gamma_{ij_l}^{(T)}$ and $|\Gamma_{ij_l}^{(T)}|$ the length of $\Gamma_{ij_l}^{(T)}$. For $T \in \mathcal{T}_h$ and $M_i \in T$, we have:

$$\sum_{l=1}^2 |\Gamma_{ij_l}^{(T)}| \mathbf{n}_{ij_l}^{(T)} = -|T| \nabla \psi_i, \quad (3)$$

where ψ_i is the \mathbb{P}_1 basis function associated to the vertex M_i of T . For every $\mathcal{C}_i \in \mathcal{C}_h$, the boundary of \mathcal{C}_i is

$$\partial \mathcal{C}_i = \bigcup_{T, M_i \in T} \left(\Gamma_{ij_1}^{(T)} \cup \Gamma_{ij_2}^{(T)} \right). \quad (4)$$

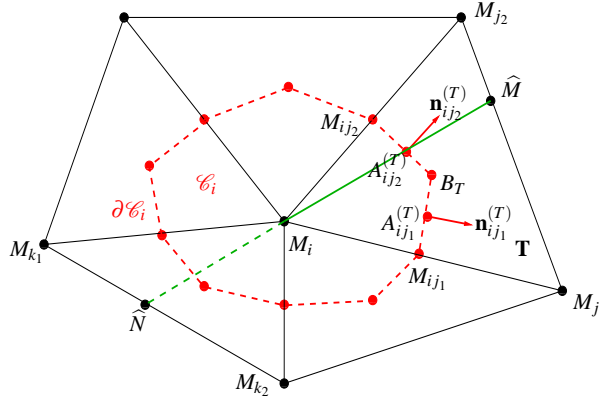


Fig. 1 Dual mesh-Vertex based control volume \mathcal{C}_i around the node M_i .

IMEX-BDF2 finite volume scheme. Here, we describe the finite volume scheme for solving (2). In order to obtain the density reconstruction on the interfaces $\Gamma_{ij_l}^{(T)}$, we use the MUSCL technique with a multislope gradient reconstruction. Concerning the time discretization, we adapt the implicit-explicit (IMEX) linear 2-step methods using *extrapolated BDF2* scheme for the convective term combined with *implicit BDF2* scheme for the diffusive term. The velocity field $\mathbf{u}(t, \mathbf{x}) \in \mathbb{R}^2$ is a given function verifying the divergence free condition. For the space discretization, the usual vertex-based finite volume scheme on control volume \mathcal{C}_i , for all $i \in [1, I]$, reads

$$\frac{d}{dt} \int_{\mathcal{C}_i} \rho(t, \mathbf{x}) d\mathbf{x} + \int_{\partial\mathcal{C}_i} \rho(t, \mathbf{x}) \mathbf{u}(t, \mathbf{x}) \cdot \mathbf{n} d\sigma = \lambda \int_{\partial\mathcal{C}_i} \nabla \rho(t, \mathbf{x}) \cdot \mathbf{n} d\sigma. \quad (5)$$

We denote by Δt the time step and $t^n = n\Delta t$, $n \geq 0$, but variable time steps can also be used. Then, the approximate solution ρ_i^n , $i \in [1, I]$, at time t^n , verifies

$$\rho_i^n \approx \frac{1}{|\mathcal{C}_i|} \int_{\mathcal{C}_i} \rho(t^n, \mathbf{x}) d\mathbf{x}.$$

In particular, the numerical approximation of the density is a piecewise constant function in space on the control volume \mathcal{C}_i . For the time discretization, we consider the implicit BDF2 scheme and an extrapolated BDF2 scheme following [10]. With this choice, we obtain a second-order accuracy in time. Then, the equation (5) is rewritten as follows, for each $i \in [1, I]$ and $n \geq 1$,

$$\begin{aligned} \rho_i^{n+1} - \frac{2\lambda}{3} \frac{\Delta t}{|\mathcal{C}_i|} \int_{\partial\mathcal{C}_i} \nabla \rho(t^{n+1}, \mathbf{x}) \cdot \mathbf{n} d\sigma &= \frac{4}{3} \rho_i^n - \frac{4}{3} \frac{\Delta t}{|\mathcal{C}_i|} \int_{\partial\mathcal{C}_i} \rho(t^n, \mathbf{x}) \mathbf{u}(t^n, \mathbf{x}) \cdot \mathbf{n} d\sigma \\ &\quad - \frac{1}{3} \rho_i^{n-1} + \frac{2}{3} \frac{\Delta t}{|\mathcal{C}_i|} \int_{\partial\mathcal{C}_i} \rho(t^{n-1}, \mathbf{x}) \mathbf{u}(t^{n-1}, \mathbf{x}) \cdot \mathbf{n} d\sigma. \end{aligned} \quad (6)$$

In order to approximate $\nabla \rho(t^{n+1}, \mathbf{x})$ in (6), we consider a \mathbb{P}_1 -finite element approach for the density such that

$$\rho|_T^{n+1} \approx \sum_{M_j \in T} \psi_j \rho_j^{n+1}, \quad \text{for all } T \in \mathcal{T}_h,$$

with $\{\psi_j\}_{j \in [1, I]}$ the canonical basis of the usual \mathbb{P}_1 finite element space. Using (3) and (4), we find ρ_i^{n+1} , $i \in [1, I]$, $n \geq 1$, verifying the following second-order *IMEX-BDF2 finite volume scheme*:

$$\begin{aligned} \rho_i^{n+1} + \frac{2\lambda}{3} \frac{\Delta t}{|\mathcal{C}_i|} \sum_{T, M_i \in T} |T| \sum_{M_j \in T} \nabla \psi_i \cdot \nabla \psi_j \rho_j^{n+1} \\ = \frac{4}{3} \rho_i^n - \frac{4}{3} \frac{\Delta t}{|\mathcal{C}_i|} \sum_{T, M_i \in T} \sum_{l=1}^2 |\Gamma_{ij_l}^{(T)}| G_{ij_l}^n(\rho_{ij_l}^n, \rho_{j_l i}^n) \\ - \frac{1}{3} \rho_i^{n-1} + \frac{2}{3} \frac{\Delta t}{|\mathcal{C}_i|} \sum_{T, M_i \in T} \sum_{l=1}^2 |\Gamma_{ij_l}^{(T)}| G_{ij_l}^{n-1}(\rho_{ij_l}^{n-1}, \rho_{j_l i}^{n-1}). \end{aligned} \quad (7)$$

Here we denote by $G_{ij_l}(\rho_1, \rho_2)$ a numerical flux that satisfies the consistency, conservativity and monotonicity properties. In particular, for any constant function ρ_1 , we have

$$\sum_{k \in \mathcal{V}(i)} |\Gamma_{ik}^{(T)}| G_{ik}(\rho_1, \rho_1) = 0. \quad (8)$$

In [2], G_{ij_l} is the upstream flux, but many other numerical fluxes can be considered, as for instance Lax-Friedrichs or Engquist-Osher fluxes. We underline that for multi-

physics coupled models, a particular attention must be paid in the approximation of the continuous velocity associated to any point of $\partial\mathcal{C}_i$ (see [3]).

In (7), ρ_{ij_l} and ρ_{ji} denote the density reconstructions on the segments $\Gamma_{ij_l}^{(T)}$, for $l = 1, 2$. In order to reach a second-order accuracy in space, we use the MUSCL technique [13] with a multislope gradient reconstruction. Introducing $\widehat{M} = [M_{j_1} M_{j_2}] \cap (M_i A_{ij_l}^{(T)})$ and $\widehat{N} \in [M_{k_1} M_{k_2}] \cap (M_i A_{ij_l}^{(T)})$, we define

$$\rho_{ij_l}^{\text{up}} = \frac{\rho_i - \rho_{\widehat{N}}}{\|M_i \widehat{N}\|} \quad \text{and} \quad \rho_{ij_l}^{\text{down}} = \frac{\rho_{\widehat{M}} - \rho_i}{\|M_i \widehat{M}\|}.$$

Then, ρ_{ij_l} is the density evaluated at node $A_{ij_l}^{(T)}$, defined as:

$$\rho_{ij_l} = \rho_i + \widehat{p}_{ij_l} \|M_i A_{ij_l}^{(T)}\|, \quad \text{with} \quad \widehat{p}_{ij_l} = p_{ij_l}^{\text{up}} \text{Lim} \left(\frac{p_{ij_l}^{\text{down}}}{p_{ij_l}^{\text{up}}} \right),$$

where Lim is a so-called "τ-limiter" (for details see [2]). In particular, they have the following result:

Lemma 1. *There exists some coefficients $\omega_{ij_l k} \geq 0$, $k \in \mathcal{V}(i)$, such that*

$$\rho_{ij_l} - \rho_i = \sum_{k \in \mathcal{V}(i)} \omega_{ij_l k} (\rho_i - \rho_k)$$

holds, and furthermore, they verify $\sum_{k \in \mathcal{V}(i)} \omega_{ij_l k} \leq \frac{7\tau}{12} C_{\mathcal{T}_h}$, where the constant $C_{\mathcal{T}_h}$ characterizes the mesh regularity (but it is more general than the classical Ciarlet ratio) and $\tau > 0$ is used in the definition of the τ-limiter.

3 L^∞ -stability of the numerical scheme

The IMEX-BDF2 finite volume scheme (7) is rewritten as linear system:

$$\mathbf{A} \boldsymbol{\rho}^{n+1} = \mathbf{F}^n, \tag{9}$$

where the matrix \mathbf{A} and the right hand side \mathbf{F}^n are defined as follows:

$$\begin{aligned} A_{i,i} &= 1 + 2\lambda \Delta t \sum_{T, M_i \in T} \|\nabla \psi_i\|^2, \quad A_{i,j} = 2\lambda \Delta t \sum_{T, M_i \neq M_j \in T} \nabla \psi_i \cdot \nabla \psi_j, \quad \forall i, j \in [1, I], \\ F_i^n &= \frac{4}{3} \rho_i^n - \frac{4}{3} \frac{\Delta t}{|\mathcal{C}_i|} \sum_{T, M_i \in T} \sum_{l=1}^2 |\Gamma_{ij_l}^{(T)}| G_{ij_l}^n(\rho_{ij_l}^n, \rho_{ji}^n) \\ &\quad - \frac{1}{3} \rho_i^{n-1} + \frac{2}{3} \frac{\Delta t}{|\mathcal{C}_i|} \sum_{T, M_i \in T} \sum_{l=1}^2 |\Gamma_{ij_l}^{(T)}| G_{ij_l}^{n-1}(\rho_{ij_l}^{n-1}, \rho_{ji}^{n-1}), \quad \forall i \in [1, I]. \end{aligned}$$

Under the hypotheses (H1) and (H2) on the mesh \mathcal{T}_h , the matrix \mathbf{A} is an M-matrix.

Remark 1. The hypothesis (H2), necessary to establish error estimates, is classical for the vertex-centered finite volume scheme [12] or the combined finite volume-finite element scheme [9]. Obviously, the M-matrix property still holds for Delaunay triangulations (see [6], Sect. 3.4).

Now, we prove the following result:

Proposition 1. *If for any $n \geq 1$, we have $\rho^{n-1} \geq 0$ and $\rho^n \geq 0$, then the right hand side of linear system (9) satisfy $\mathbf{F}^n \geq 0$ under the CFL condition:*

$$\Delta t \leq \min_{1 \leq i \leq I} \frac{|\mathcal{C}_i|}{\frac{2}{3} \left(\frac{7\tau}{12} C_{\mathcal{F}_h} + 2 \right) \|\mathbf{u}\|_{i,\infty} \sum_{T, M_i \in T} \left(|\Gamma_{ij_1}^{(T)}| + |\Gamma_{ij_2}^{(T)}| \right)}, \quad (10)$$

with $\|\mathbf{u}\|_{i,\infty} = \max_{T, M_i \in T} \|\mathbf{u}_T\|_{l^2(\mathbb{R}^2)}$ where \mathbf{u}_T is the cell average velocity.

Proof. Let $i \in [1, I]$ and $n \geq 1$. Thanks to (8), the i -th row of (9) is given by:

$$\begin{aligned} \left(\mathbf{A} \rho^{n+1} \right)_i &= \frac{4}{3} \rho_i^n - \frac{4}{3} \frac{\Delta t}{|\mathcal{C}_i|} \sum_{T, M_i \in T} \sum_{l=1}^2 |\Gamma_{ij_l}^{(T)}| \left(G_{ij_l}^n(\rho_{ij_l}^n, \rho_{j_l i}^n) - G_{ij_l}^n(\rho_i^n, \rho_i^n) \right) \\ &- \frac{1}{3} \rho_i^{n-1} + \frac{2}{3} \frac{\Delta t}{|\mathcal{C}_i|} \sum_{T, M_i \in T} \sum_{l=1}^2 |\Gamma_{ij_l}^{(T)}| \left(G_{ij_l}^{n-1}(\rho_{ij_l}^{n-1}, \rho_{j_l i}^{n-1}) - G_{ij_l}^{n-1}(\rho_i^{n-1}, \rho_i^{n-1}) \right). \end{aligned} \quad (11)$$

Let us introduce some definitions and notations dropping the time indices, such that

$$\Delta \rho_{ij_l} = \rho_{ij_l} - \rho_i, \quad \tilde{\Delta} \rho_{ij_l} = \rho_{j_l i} - \rho_i, \quad \text{for } l = 1, 2.$$

Thanks to Lemma 1, there exists for $l = 1, 2$, some coefficients $\omega_{ijk} \geq 0$, $k \in \mathcal{V}(i)$, such that

$$\Delta \rho_{ij_l} = \sum_{k \in \mathcal{V}(i)} \omega_{ijk} (\rho_i - \rho_k), \quad \text{with } \sum_{k \in \mathcal{V}(i)} \omega_{ijk} \leq \frac{7\tau}{12} C_{\mathcal{F}_h}.$$

Also, there exists for $l = 1, 2$, some coefficients $\tilde{\omega}_{ijk} \geq 0$, $k \in \mathcal{V}(i)$, such that

$$\tilde{\Delta} \rho_{ij_l} = \sum_{k \in \mathcal{V}(i)} \tilde{\omega}_{ijk} (\rho_k - \rho_i), \quad \text{with } \sum_{k \in \mathcal{V}(i)} \tilde{\omega}_{ijk} \leq 2.$$

Next, for $0 < \delta_{ij_l} < 1$, $l = 1, 2$, we consider the following quantities:

$$\begin{aligned} E_{ij_l} &= \frac{|\Gamma_{ij_l}^{(T)}|}{|\mathcal{C}_i|} \frac{\partial G_{ij_l}}{\partial \rho_1} (\rho_i + \delta_{ij_l} \Delta \rho_{ij_l}, \rho_i + \delta_{ij_l} \tilde{\Delta} \rho_{ij_l}), \quad l = 1, 2, \\ F_{ij_l} &= -\frac{|\Gamma_{ij_l}^{(T)}|}{|\mathcal{C}_i|} \frac{\partial G_{ij_l}}{\partial \rho_2} (\rho_i + \delta_{ij_l} \Delta \rho_{ij_l}, \rho_i + \delta_{ij_l} \tilde{\Delta} \rho_{ij_l}), \quad l = 1, 2. \end{aligned}$$

Of course, by monotonicity of the numerical flux, we have $E_{ij_l} \geq 0$ and $F_{ij_l} \geq 0$. Hence, using the mean value theorem, the numerical scheme (11) is rewritten as

follows:

$$\begin{aligned} (\mathbf{A}\rho^{n+1})_i &= \frac{4}{3}\rho_i^n - \frac{4}{3}\Delta t \sum_{T, M_i \in T} \sum_{k \in \mathcal{V}(i)} \sum_{l=1}^2 \left(\omega_{ijlk} \mathbf{E}_{ijl}^n (\rho_i^n - \rho_k^n) - \tilde{\omega}_{ijlk} \mathbf{F}_{ijl}^n (\rho_k^n - \rho_i^n) \right) \\ &- \frac{1}{3}\rho_i^{n-1} + \frac{2}{3}\Delta t \sum_{T, M_i \in T} \sum_{k \in \mathcal{V}(i)} \sum_{l=1}^2 \left(\omega_{ijlk} \mathbf{E}_{ijl}^{n-1} (\rho_i^{n-1} - \rho_k^{n-1}) - \tilde{\omega}_{ijlk} \mathbf{F}_{ijl}^{n-1} (\rho_k^{n-1} - \rho_i^{n-1}) \right). \end{aligned} \quad (12)$$

Finally, we obtain the following equations for each $i \in [1, I]$ and for all $n \geq 1$:

$$(\mathbf{A}\rho^{n+1})_i = a_{ii} \rho_i^n + b_{ii} \rho_i^{n-1} + \sum_{k \in \mathcal{V}(i)} (a_{ik} \rho_k^n + b_{ik} \rho_k^{n-1}), \quad (13)$$

where a_{ii} , b_{ii} , a_{ik} and b_{ik} are easily determined from (12). Clearly, we have

$$a_{ii} + b_{ii} + \sum_{k \in \mathcal{V}(i)} (a_{ik} + b_{ik}) = 1. \quad (14)$$

Moreover, by choosing the time step Δt such that for all $i \in [1, I]$,

$$\Delta t \leq \left(\sum_{T, M_i \in T} \sum_{k \in \mathcal{V}(i)} \sum_{l=1}^2 \left(\frac{4}{3} (\omega_{ijlk} \mathbf{E}_{ijl}^n + \tilde{\omega}_{ijlk} \mathbf{F}_{ijl}^n) - \frac{2}{3} (\omega_{ijlk} \mathbf{E}_{ijl}^{n-1} + \tilde{\omega}_{ijlk} \mathbf{F}_{ijl}^{n-1}) \right) \right)^{-1}, \quad (15)$$

we have

$$0 \leq a_{ii} + b_{ii} \leq 1 \quad \text{and} \quad 0 \leq a_{ik} + b_{ik} \leq 1. \quad (16)$$

Hence, (13), (14) and (16) allow us to conclude that for each $i \in [1, I]$, $(\mathbf{A}\rho^{n+1})_i$ is written as convex combination of ρ_i^n , ρ_i^{n-1} , ρ_k^n and ρ_k^{n-1} , $k \in \mathcal{V}(i)$. \square

Finally, as a consequence of Proposition 1, and recalling that an M-matrix is invertible with positive inverse, we obtain:

Theorem 1. *Let the velocity field \mathbf{u} divergence free and the initial density ρ_0 such that $\rho_0(x) \geq 0$. Then, under the CFL condition (10) and the hypotheses (H1) and (H2) on the mesh, the linear system (9) is invertible, and*

$$\rho^{n+1} \geq 0, \quad \forall n \geq 1. \quad (17)$$

Numerical results. Here we consider structured meshes on $\Omega =]-1, 1[^2$, a stationary rotating velocity field $\mathbf{u} = (x_2, -x_1)$ and a small diffusion coefficient $\lambda = 10^{-6}$. Setting $r = \sqrt{(x_1 + 0.5)^2 + x_2^2}$, the discontinuous initial condition is $\rho_0 = 1000$ if $r \leq 0.25$ and $\rho_0 = 1$ if $r > 0.25$. The computations are performed for different values of $h \geq 0.004$, until $T = 0.3$. In Fig. 2 we show the evolution of the density contours (left) and the solution profiles for some horizontal sections (right). We can remark that the maximum principle is well verified using the IMEX-BDF2 scheme, unlike other classical order two schemes, such as Crank-Nicolson Adams-Bashforth or Crank-Nicolson Runge-Kutta. Some other numerical results can be found in [7].

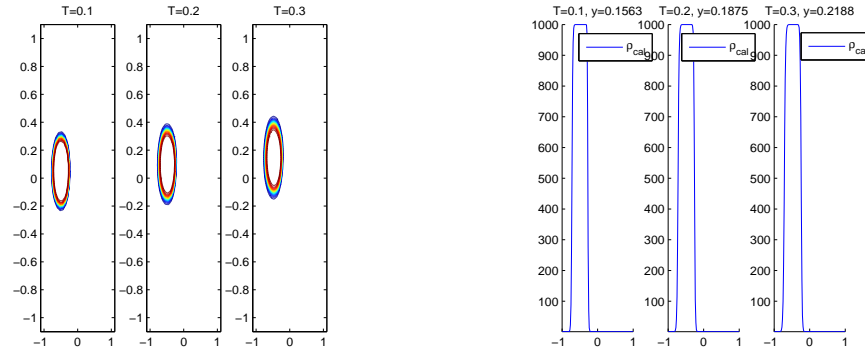


Fig. 2 The evolution of the density contours (left) and the solution profiles (right) for $\lambda = 10^{-6}$.

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