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$L^\infty$-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, $L^\infty$-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 $v$ (which is not solenoidal) and the pressure $p$. Following Kazhikhov and Smagulov [11], we set

$$u = v + \lambda \nabla \ln(\rho),$$

(1)

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Caterina Calgaro
Univ. Lille, CNRS, UMR 8524 - Laboratoire Paul Painlevé,
F-59000 Lille, France
e-mail: caterina.calgaro@univ-lille1.fr

Meriem Ezzoug
UR: Multifractals et Ondelettes. FSM. Université de Monastir. 5019 Monastir, Tunisie
ISSIG. Université de Gabès. 6032 Gabès, Tunisie
e-mail: meriemezzoug@yahoo.fr
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 $\text{div}\mathbf{u} = 0$ and we obtain the non-standard constraint $\text{div}\mathbf{v} = -\text{div}(\lambda \nabla \ln(\rho))$, which is relied on the definition of the pressure $p$. Using (1), the mass conservation equation becomes

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

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 $L^\infty$-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 $\Omega$ 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 $\Omega$ 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 $\Omega$.
(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 $M_i, M_{j1}, M_{j2}$ the three vertices of $T$. We also denote respectively $M_{ij1}$ and $M_{ij2}$ the middles of $[M_iM_{j1}]$ and $[M_iM_{j2}]$.

Let us construct the dual mesh $\mathcal{C}_h = \{\mathcal{C}_i, i \in [1, I]\}$, which defines a second partition of $\Omega$. ($I \in \mathbb{N}^*$ 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 \( \bigcup_{T \in \mathcal{F}_h} T = \tilde{\Omega} = \bigcup_{i \in [1,I]} \mathcal{C}_i \).

Moreover, if we denote \( |\mathcal{C}_i| \) the area of \( \mathcal{C}_i \in \mathcal{G}_h \), 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 \( \Gamma_{i,l}^{(T)} = \text{the segment } [M_{i,l},B_T] \), \( A_{i,l}^{(T)} \) its middle point, \( n_{i,l}^{(T)} \) the unit outward normal to \( \mathcal{C}_i \) along \( \Gamma_{i,l}^{(T)} \) and \( |\Gamma_{i,l}^{(T)}| \) the length of \( \Gamma_{i,l}^{(T)} \). For \( T \in \mathcal{F}_h \) and \( M_i \in T \), we have:

\[
\sum_{l=1}^{2} |\Gamma_{i,l}^{(T)}| n_{i,l}^{(T)} = -|T| \nabla \psi_i, \tag{3}
\]

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

\[
\partial \mathcal{C}_i = \bigcup_{T,M_i \in T} \left( \Gamma_{i,1}^{(T)} \cup \Gamma_{i,2}^{(T)} \right). \tag{4}
\]

**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 \( \Gamma_{i,l}^{(T)} \), 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 \( \mathbf{u}(t,x) \in \mathbb{R}^2 \) 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
We denote by $\Delta t$ the time step and $t^n = n\Delta t$, $n \geq 0$, but variable time steps can also be used. Then, the approximate solution $\rho^n_i$, $i \in [1, I]$, at time $t^n$, verifies

$$\rho^n_i \approx \frac{1}{|G_i|} \int_{G_i} \rho(t^n, x) \, dx.$$ 

In particular, the numerical approximation of the density is a piecewise constant function in space on the control volume $G_i$. 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 $n \geq 1$,

$$\rho^n_i + \frac{2\lambda}{3} \frac{\Delta t}{|G_i|} \int_{\partial G_i} \nabla \rho(t^{n+1}, x) \cdot \mathbf{n} \, d\sigma = \frac{4}{3} \rho^n_i - \frac{4}{3} \frac{\Delta t}{|G_i|} \int_{\partial G_i} \rho(t^n, x) \mathbf{u}(t^n, x) \cdot \mathbf{n} \, d\sigma$$

$$\quad - \frac{1}{3} \rho_{i-1}^n + \frac{2}{3} \frac{\Delta t}{|G_i|} \int_{\partial G_i} \rho(t^{n-1}, x) \mathbf{u}(t^{n-1}, x) \cdot \mathbf{n} \, d\sigma.$$ 

In order to approximate $\nabla \rho(t^{n+1}, x)$ in (6), we consider a $P_1$-finite element approach for the density such that

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

with $\{ \psi_j \}_{j \in [1, I]}$ the canonical basis of the usual $P_1$ finite element space. Using (3) and (4), we find $\rho^n_{i+1}, i \in [1, I], n \geq 1$, verifying the following second-order IMEX-BDF2 finite volume scheme:

$$\rho^n_{i+1} + \frac{2\lambda}{3} \frac{\Delta t}{|G_i|} \sum_{T, M_j \in T} \left| T \right| \sum_{M_j \in T} \nabla \psi_i \cdot \nabla \psi_j \rho^n_{j+1}$$

$$= \frac{4}{3} \rho^n_i - \frac{4}{3} \frac{\Delta t}{|G_i|} \sum_{T, M_j \in T} \sum_{T_i=1}^{2} |G_{ij}^{(T)}| G_{ij}^{n} \left( \rho^n_i, \rho^n_{j+1} \right)$$

$$- \frac{1}{3} \rho_{i-1}^n + \frac{2}{3} \frac{\Delta t}{|G_i|} \sum_{T, M_j \in T} \sum_{T_i=1}^{2} |G_{ij}^{(T)}| G_{ij}^{n-1} \left( \rho^n_{j-1}, \rho^n_{j+1} \right).$$ 

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

$$\sum_{k \in T} |G_{ik}^{(T)}| G_{ik} \left( \rho_1, \rho_1 \right) = 0.$$ 

In [2], $G_{ij}$ 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 \(\partial\Omega_h\) (see [3]).

In (7), \(\rho_{ij}\) and \(\rho_{ji}\) denote the density reconstructions on the segments \(\Gamma_{ij}^{(T)}\), 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 \(\mathcal{M} = [M_k, M_{ij}] \cap (M_iA_{ij}^{(T)})\) and \(\tilde{N} \in [M_k, M_{k2}] \cap (M_iA_{ij}^{(T)})\), we define

\[
p_{ij}^{\text{up}} = \frac{\rho_i - \rho_{\tilde{N}}}{\|M_iN\|} \quad \text{and} \quad p_{ij}^{\text{down}} = \frac{\rho_M - \rho_i}{\|M_iM\|}
\]

Then, \(\rho_{ij}\) is the density evaluated at node \(A_{ij}^{(T)}\), defined as:

\[
\rho_{ij} = \rho_i + \rho_{\tilde{ij}} \|M_iA_{ij}^{(T)}\|, \quad \text{with} \quad \rho_{\tilde{ij}} = \rho_{ij}^{\text{up}} \text{Lim}\left(\frac{p_{ij}^{\text{down}}}{p_{ij}^{\text{up}}}\right),
\]

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

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

\[
\rho_{ij} - \rho_i = \sum_{k \in \mathcal{T}(i)} \omega_{ijk} (\rho_i - \rho_k)
\]

holds, and furthermore, they verify \(\sum_{k \in \mathcal{T}(i)} \omega_{ijk} \leq \frac{2}{\tau} C_{\mathcal{R}_h}\), where the constant \(C_{\mathcal{R}_h}\) characterizes the mesh regularity (but it is more general than the classical Ciarlet ratio) and \(\tau > 0\) is used in the definition of the \(\tau\)-limiter.

### 3 \(L^\infty\)-stability of the numerical scheme

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

\[
A \rho^{n+1} = F^n,
\]

where the matrix \(A\) and the right hand side \(F^n\) are defined as follows:

\[
A_{ij} = 1 + 2\lambda \Delta t \sum_{T,M \in \mathcal{T}} \|\nabla \psi_i\|^2, \quad A_{ij} = 2\lambda \Delta t \sum_{T,M \neq M_j \in \mathcal{T}} \nabla \psi_i \cdot \nabla \psi_j, \quad \forall i, j \in [1, I],
\]

\[
F_i^n = \frac{4}{3} \rho_i^n - \frac{4}{3} \frac{\Delta t}{|\mathcal{E}_i|} \sum_{T,M \in \mathcal{T}} \sum_{l=1}^2 |I_{ij}^{(T)}| G_{ij}^n (\rho_{ij}^n, \rho_{ji}^n) - \frac{1}{3} \rho_i^{n-1} + \frac{2}{3} \frac{\Delta t}{|\mathcal{E}_i|} \sum_{T,M \in \mathcal{T}} \sum_{l=1}^2 |I_{ij}^{(T)}| G_{ij}^{n-1} (\rho_{ij}^{n-1}, \rho_{ji}^{n-1}), \quad \forall i \in [1, I].
\]

Under the hypotheses (H1) and (H2) on the mesh \(\mathcal{H}_h\), the matrix \(A\) 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 \( F^n \geq 0 \) under the CFL condition:

\[
\Delta t \leq \min_{1 \leq i \leq l} \frac{2 \left( \frac{7\tau}{12} C_{\mathcal{G}_h} + 2 \right) \| u \|_{i,\infty}}{\sum_{T, M \in T} \left( |G_{ij}^{(T)}| + |G_{ij}^{(T)}| \right) },
\]

with \( \| u \|_{i,\infty} = \max_{T, M \in T} \| u_{ij} \| \infty \) where \( u_{ij} \) is the cell average velocity.

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

\[
\begin{align*}
(A \rho^{n+1})_i &= \frac{4}{3} \rho^n_i \frac{4 \Delta t}{3 |\mathcal{G}_i|} \sum_{T, M \in T} \sum_{l=1}^2 \int_{T_{ij}} \left( G_{ij}^{(T)}(\rho_{ij}^n, \rho_{ij}^n) - G_{ij}^{(T)}(\rho_{ij}^n, \rho_{ij}^n) \right) \nonumber \\
&- \frac{1}{3} \rho^n_i + \frac{2 \Delta t}{3 |\mathcal{G}_i|} \sum_{T, M \in T} \sum_{l=1}^2 \int_{T_{ij}} \left( G_{ij}^{a-1}(\rho_{ij}^{a-1}, \rho_{ij}^{a-1}) - G_{ij}^{a-1}(\rho_{ij}^{a-1}, \rho_{ij}^{a-1}) \right).
\end{align*}
\]

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

\[
\Delta \rho_{ij} = \rho_{ij} - \rho_i, \quad \tilde{\Delta} \rho_{ij} = \rho_{ij} - \rho_i, \quad \text{for } l = 1, 2.
\]

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

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

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

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

Next, for \( 0 < \delta_{ij} < 1, l = 1, 2 \), we consider the following quantities:

\[
E_{ij} = \frac{|G_{ij}^{(T)}|}{|\mathcal{G}_i|} \frac{\partial G_{ij}}{\partial \rho_1}(\rho_i + \delta_{ij} \Delta \rho_{ij}, \rho_i + \delta_{ij} \tilde{\Delta} \rho_{ij}), \quad l = 1, 2,
\]

\[
F_{ij} = -\frac{|G_{ij}^{(T)}|}{|\mathcal{G}_i|} \frac{\partial G_{ij}}{\partial \rho_2}(\rho_i + \delta_{ij} \Delta \rho_{ij}, \rho_i + \delta_{ij} \tilde{\Delta} \rho_{ij}), \quad l = 1, 2.
\]

Of course, by monotonicity of the numerical flux, we have \( E_{ij} \geq 0 \) and \( F_{ij} \geq 0 \). Hence, using the mean value theorem, the numerical scheme (11) is rewritten as
follows:
\[
(A\rho^{n+1})_i = \frac{4}{3}\rho_i^n - \frac{4}{3}\Delta t \sum_{T,M \in T} \sum_{k \in \mathcal{Y}(i)} \left( \sum_{l=1}^2 \left( a_{ijkl} E^n_{ijl} (\rho_i^n - \rho_k^n) - \tilde{a}_{ijkl} F^n_{ijl} (\rho_i^n - \rho_k^n) \right) \right)
- \frac{1}{3}\rho_i^{n-1} + \frac{2}{3}\Delta t \sum_{T,M \in T} \sum_{k \in \mathcal{Y}(i)} \left( \sum_{l=1}^2 \left( a_{ijkl} E^{n-1}_{ijl} (\rho_i^{n-1} - \rho_k^{n-1}) - \tilde{a}_{ijkl} F^{n-1}_{ijl} (\rho_i^{n-1} - \rho_k^{n-1}) \right) \right).
\]

Finally, we obtain the following equations for each \( i \in [1, I] \) and for all \( n \geq 1 \):
\[
(A\rho^{n+1})_i = a_{ii} \rho_i^n + b_{ii} \rho_i^{n-1} + \sum_{k \in \mathcal{Y}(i)} (a_{ik} \rho_k^n + b_{ik} \rho_k^{n-1}),
\]
where \( a_{ii}, b_{ii}, a_{ik} \) and \( b_{ik} \) are easily determined from (12). Clearly, we have
\[
a_{ii} + b_{ii} + \sum_{k \in \mathcal{Y}(i)} (a_{ik} + b_{ik}) = 1.
\]
Moreover, by choosing the time step \( \Delta t \) such that for all \( i \in [1, I] \),
\[
\Delta t \leq \frac{1}{\sum_{T,M \in T} \sum_{k \in \mathcal{Y}(i)} \left( \frac{4}{3}(a_{ijkl} E^n_{ijl} + \tilde{a}_{ijkl} F^n_{ijl}) \right) - \frac{2}{3}(a_{ijkl} E^{n-1}_{ijl} + \tilde{a}_{ijkl} F^{n-1}_{ijl})}},
\]
we have
\[
0 \leq a_{ii} + b_{ii} \leq 1 \quad \text{and} \quad 0 \leq a_{ik} + b_{ik} \leq 1.
\]
Hence, (13), (14) and (16) allow us to conclude that for each \( i \in [1, I] \), \((A\rho^{n+1})_i\) is written as convex combination of \( \rho_i^n, \rho_i^{n-1}, \rho_k^n \) and \( \rho_k^{n-1} \), \( k \in \mathcal{Y}(i) \).

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 \( u \) divergence free and the initial density \( \rho_0 \) 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
\[
\rho^{n+1} \geq 0, \quad \forall \ n \geq 1.
\]

**Numerical results.** Here we consider structured meshes on \( \Omega = [-1,1]^2 \), a stationary rotating velocity field \( u = (x_2, -x_1) \) 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 $\lambda = 10^{-6}$.

References