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CONSERVATION SCHEMES FOR CONVECTION-DIFFUSION EQUATIONS WITH ROBIN'S BOUNDARY CONDITIONS *

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Abstract. A standard numerical method in order to approach the solution of a time dependent convection-diffusion equation in φ transported with velocity \mathbf{u} , consists to multiply the full equation by a space dependent test function ψ , to integrate it on the computational domain Ω , and to discretize it in space with a finite element method and in time with a finite difference scheme. The diffusion term is integrated by part on Ω but not the advected term $\mathbf{u} \cdot \nabla \varphi$. In the convection dominated regime, a streamline upwind method SUPG is used in order to stabilize the numerical scheme. In principle, when the flow is incompressible and confined in Ω , i.e. when $\operatorname{div}(\mathbf{u}) = 0$ in Ω and $\mathbf{u} \cdot \mathbf{n} = 0$ on the boundary $\partial\Omega$, the integral of φ on the domain Ω remains constant in time when the source term is vanishing (conservation of the mass balance) and when Neumann boundary conditions are applied on the boundary. Moreover, when Robin's boundary conditions are applied on the boundary $\partial\Omega$, as for example in a convection-diffusion thermal problem, an energy mass balance can be established by taking into account the energy crossing through $\partial\Omega$. However, on a practical point of view, the velocity \mathbf{u} is often computed with a Navier-Stokes solver which leads to an approximation \mathbf{u}_h which is not exactly with divergence free. As an unwelcome numerical effect, the mass balance or the energy balance are not conserved when the time goes up. Especially these defects can be important when the equation is integrated on a long time. In this paper, we propose an original modification of the standard numerical scheme in order to eliminate this defect which appears when Neumann or Robin's boundary conditions for φ are imposed on $\partial\Omega$. Moreover we show that this scheme is L^2 -stable and allows to obtain a constant stationary solution when the source term is vanishing. We also establish some error estimates produced by this new scheme.

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1. SITUATION OF THE PROBLEM

Let us assume that in a cavity $\Omega \subset \mathbb{R}^3$, in which flows an incompressible fluid with velocity \mathbf{u} depending on $t \in (0, \infty)$ and $\mathbf{x} \in \Omega$, a chemical product with concentration or a temperature field φ is convected and diffused.

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If $\partial\Omega$ is the boundary of Ω supposed bounded and Lipschitzian, and if \mathbf{n} is its external unit normal, we will assume that

$$\operatorname{div}(\mathbf{u}) = 0 \text{ in } \Omega \text{ and } \mathbf{u} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega, \quad (1)$$

where $\mathbf{u} \cdot \mathbf{n}$ is the Euclidian scalar product of \mathbf{u} with \mathbf{n} .

The convection-diffusion equation for φ is given by:

$$\partial\varphi/\partial t - \epsilon\Delta\varphi + \mathbf{u} \cdot \nabla\varphi = f \text{ in } (0, +\infty) \times \Omega, \quad (2)$$

with Robin's boundary condition:

$$\epsilon\partial\varphi/\partial n = \alpha(\varphi_r - \varphi) \text{ on } \partial\Omega, \quad (3)$$

and initial condition

$$\varphi = \varphi^0 \text{ at time } t = 0, \quad (4)$$

where φ_r is a given constant number and α is a non negative parameter. In Equation (2), f is a source term which is a priori depending on $t \in (0, +\infty)$ and $\mathbf{x} \in \Omega$, and $\epsilon > 0$ is the diffusion coefficient.

Let us remark that it is not restrictive to assume that $\varphi_r = 0$ since it suffices to change the unknown φ onto $(\varphi - \varphi_r)$. In all the sequel we will assume that $\varphi_r = 0$.

On a mathematical point of view we assume that T is the final time and that $f \in L^2((0, T) \times \Omega)$ and $\varphi^0 \in L^2(\Omega)$. Using the standard notations for Sobolev spaces $H^1(\Omega)$, $H^2(\Omega)$, $H^1((0, T); L^2(\Omega))$, $C^1([0, T]; L^2(\Omega))$... (see [3], [10]), we suppose that $\mathbf{u} \in H^2(\Omega)$ is given and not depending on t (in fact it is not difficult to adapt the following to the case where \mathbf{u} is depending on t).

A classical weak formulation of (2)-(3) with $\varphi_r = 0$ (see [3], [8]) consists to look for $\varphi \in L^2((0, T); H^1(\Omega)) \cap C^0([0, T]; L^2(\Omega))$ satisfying for every $\psi \in H^1(\Omega)$:

$$\int_{\Omega} \frac{\partial\varphi}{\partial t} \psi dx + \epsilon \int_{\Omega} \nabla\varphi \cdot \nabla\psi dx + \alpha \int_{\partial\Omega} \varphi \psi ds + \int_{\Omega} (\mathbf{u} \cdot \nabla\varphi) \psi dx = \int_{\Omega} f \psi dx. \quad (5)$$

Since we have assumed that $\operatorname{div}(\mathbf{u}) = 0$, then $\mathbf{u} \cdot \nabla\varphi = \operatorname{div}(\mathbf{u}\varphi)$ and $(\mathbf{u} \cdot \nabla\varphi)\varphi = \frac{1}{2} \operatorname{div}(\mathbf{u}\varphi^2)$. Moreover with $\mathbf{u} \cdot \mathbf{n} = 0$ on $\partial\Omega$, we obtain by using the divergence theorem:

Property 1: If $\psi = 1$ in (5), we have:

$$\frac{d}{dt} \int_{\Omega} \varphi dx + \alpha \int_{\partial\Omega} \varphi ds = \int_{\Omega} f dx. \quad (6)$$

Property 2: If $\psi = \varphi$ in (5), we have:

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} \varphi^2 dx + \epsilon \int_{\Omega} |\nabla\varphi|^2 dx + \alpha \int_{\partial\Omega} \varphi^2 ds = \int_{\Omega} f \varphi dx. \quad (7)$$

Property 3:

$$\text{if } \alpha = 0 \text{ and } f = 0, \text{ then } \lim_{t \rightarrow \infty} \varphi = \text{const.} \quad (8)$$

Property 1 is important since it is describing the conservation of the thermal energy if φ is a temperature variable or the conservation of the mass of material if φ is a density variable. For example if the source term is

vanishing and if the physical system is isolated ($f = 0$ and $\alpha = 0$), the integral of φ on Ω remains constant in time (conservation of total energy or conservation of total mass in Ω , i.e. $\int_{\Omega} \varphi dx = \int_{\Omega} \varphi^0 dx$ for every $t > 0$)

Property 2 is also important since it is a stability relation. In fact if we denote by $\|v\|$ the $L^2(\Omega)$ norm of $v \in L^2(\Omega)$ and $\|\nu\|_1 =_{def} (\epsilon \int_{\Omega} |\nabla \nu|^2 dx + \alpha \int_{\partial\Omega} |\nu|^2 ds)^{\frac{1}{2}}$ for $\nu \in H^1(\Omega)$, it is well known that if $\alpha > 0$ then $\|\cdot\|_1$ is a norm equivalent to the standard H^1 -norm and consequently we obtain from Property 2:

$$\frac{d}{dt} \|\varphi\| + \lambda_1 \|\varphi\| \leq \|f\|, \quad (9)$$

where $\lambda_1 = \inf_{\nu \in H^1(\Omega)} \frac{\|\nu\|_1}{\|\nu\|}$.

In particular if $f = 0$ and $\alpha > 0$, the L^2 -norm of the variable φ is exponentially decreasing when the time goes up ($\|\varphi\| = e^{-\lambda_1 t} \|\varphi^0\|$). In the case $\alpha = 0$ we obtain the same behavior for $\varphi - \bar{\varphi}$ where $\bar{\varphi}$ is the mean value of φ in Ω .

Finally Property 3 is also important because when $f = 0$ and $\alpha = 0$ (isolated system without source), the stationary solution $\varphi = const$ is solution of (5).

In the next section, given an approximation \mathbf{u}_h of \mathbf{u} , we would like to define a semi-discretization in space of (5) which will allow to compute an approximation φ_h of φ by keeping the above properties, i.e.

Property 1h: conservation of energy or mass:

$$\frac{d}{dt} \int_{\Omega} \varphi_h dx + \alpha \int_{\partial\Omega} \varphi_h ds = \int_{\Omega} f dx. \quad (10)$$

Property 2h: stability of the scheme:

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} \varphi_h^2 dx + \epsilon \int_{\Omega} |\nabla \varphi_h|^2 dx + \alpha \int_{\partial\Omega} \varphi_h^2 ds = \int_{\Omega} f \varphi_h dx. \quad (11)$$

Property 3h: stationary constant solution:

$$\text{if } \alpha = 0 \text{ and } f = 0, \text{ then } \varphi_h = const \text{ is a solution of (5) when } \mathbf{u} \text{ is replaced by } \mathbf{u}_h. \quad (12)$$

2. SEMI-DISCRETIZATION IN SPACE.

In order to consider a semi-discretization in space of Equation (5), we assume for the sake of simplicity, that Ω is a polygonal domain. If Γ_h is a conforming mesh of Ω in tetrahedra $K \in \Gamma_h$ with diameter h_K smaller than h , we define the standard finite element space V_h of piecewise polynomial functions $P_1(K)$ of degree 1 on K by

$$V_h = \{g : \Omega \rightarrow \mathbb{R} : g \text{ continuous and } g|_K \in \mathbb{P}_1(K), \forall K \in \Gamma_h\}. \quad (13)$$

When h_K is small with respect to $\epsilon / \|\mathbf{u}_h\|_{L_2(K)}$ for every $K \in \Gamma_h$, a standard finite element approximation scheme in space for computing an approximation φ_h of φ is to looking for a function $\varphi_h \in H^1((0, T); V_h)$ satisfying:

$$\int_{\Omega} \frac{\partial \varphi_h}{\partial t} \psi_h dx + \epsilon \int_{\Omega} \nabla \varphi_h \cdot \nabla \psi_h dx + \alpha \int_{\partial \Omega} \varphi_h \psi_h ds + \int_{\Omega} L(\mathbf{u}_h, \varphi_h, \psi_h) dx = \int_{\Omega} f \psi_h dx, \quad \forall \psi_h \in V_h, \quad (14)$$

where $\mathbf{u}_h \in V_h^3$ is obtained from a computation approximating \mathbf{u} (for example from a finite element Navier-Stokes code) and $\int_{\Omega} L(\mathbf{u}_h, \varphi_h, \psi_h) dx$ is a discretization of $\int_{\Omega} (\mathbf{u} \cdot \nabla \varphi) \psi dx$. The most popular approximation of $\int_{\Omega} (\mathbf{u} \cdot \nabla \varphi) \psi dx$ is obtained by setting $L(\mathbf{u}_h, \varphi_h, \psi_h) = (\mathbf{u}_h \cdot \nabla \varphi_h) \psi_h$.

In (14) we assume that the initial condition φ^0 is given in V_h and if it is not the case, we take a projection $\varphi_h^0 \in V_h$ of φ^0 as initial condition $\varphi_h(0)$.

Of course if h_K is greater than $\epsilon / \|\mathbf{u}_h\|_{L_2(K)}$ for some $K \in \Gamma_h$ (convection dominated regime in a neighborhood of K), an additional artificial term of type SUPG (see [4]) which is on the form

$$\omega \sum_{K \in \Gamma_h} \frac{\tau_K h_K}{2 \|\mathbf{u}_h\|_{L_2(K)}} \int_K (\mathbf{u}_h \cdot \nabla \varphi_h) (\mathbf{u}_h \cdot \nabla \psi) dx \quad (15)$$

must be added to Equation (14) in order to eliminate some spurious numerical oscillations. In (15), ω is an appropriate constant and $\tau_K = \max(0, 1 - 2\epsilon/h_K \|\mathbf{u}_h\|_{L_2(K)})$. Another possibility is to add to (14) an edge stabilization (see [5]) in order to eliminate spurious numerical oscillations. In the following we neglect the addition of these artificial terms which have no influence on our conclusions.

Remark 1. *Let us suppose that \mathbf{u}_h is an approximation of \mathbf{u} with the following property: there exists a constant C such that*

$$\|\mathbf{u} - \mathbf{u}_h\| + h \|\nabla(\mathbf{u} - \mathbf{u}_h)\| \leq Ch^2. \quad (16)$$

Even if $\text{div}(\mathbf{u}_h)$ is not vanishing but only of order h in the L^2 -norm, we would like that the trilinear functional $L : (\mathbf{u}, \varphi, \psi) \in H^1(\Omega)^3 \times H^1(\Omega) \times H^1(\Omega) \rightarrow L(\mathbf{u}, \varphi, \psi) \in \mathbb{R}$ satisfies the following properties, for consistency reasons and in order to verify (10), (11), (12):

- 1) $\int_{\Omega} L(\mathbf{u}, \varphi, \psi) dx = \int_{\Omega} (\mathbf{u} \cdot \nabla \varphi) \psi dx, \quad \forall \varphi, \psi \in H^1(\Omega),$
- 2) $\int_{\Omega} L(\mathbf{u}_h, \psi_h, 1) dx = 0 \quad \forall \psi_h \in V_h,$
- 3) $\int_{\Omega} L(\mathbf{u}_h, \psi_h, \psi_h) dx = 0 \quad \forall \psi_h \in V_h,$
- 4) $\int_{\Omega} L(\mathbf{u}_h, 1, \psi_h) dx = 0 \quad \forall \psi_h \in V_h.$

Clearly speaking, in order to satisfy the consistency relation 1), the standard versions of L for the discretization of $\int_{\Omega}(\mathbf{u} \cdot \nabla \varphi) \psi dx$ by $\int_{\Omega} L(\mathbf{u}_h, \varphi_h, \psi_h) dx$ are the following:

- a) $L(\mathbf{u}, \varphi, \psi) = (\mathbf{u} \cdot \nabla \varphi) \psi$,
- b) $L(\mathbf{u}, \varphi, \psi) = -(\mathbf{u} \cdot \nabla \psi) \varphi$,
- c) $L(\mathbf{u}, \varphi, \psi) = \operatorname{div}(\varphi \mathbf{u}) \psi$ or $L(\mathbf{u}, \varphi, \psi) = -\operatorname{div}(\psi \mathbf{u}) \varphi$
- d) $L(\mathbf{u}, \varphi, \psi) = \frac{1}{2}((\mathbf{u} \cdot \nabla \varphi) \psi - (\mathbf{u} \cdot \nabla \psi) \varphi)$.

Unfortunately, no above choice is able to satisfy the three above relations 2), 3), 4) and consequently properties 1h), 2h) and 3h) cannot be simultaneously satisfied when $\operatorname{div}(\mathbf{u}_h)$ is not exactly vanishing.

In this paper we propose the expression

$$e) L(\mathbf{u}, \varphi, \psi) = \frac{1}{2} [(\mathbf{u} \cdot \nabla \varphi)(\psi - \bar{\psi}) - (\mathbf{u} \cdot \nabla \psi)(\varphi - \bar{\varphi})]$$

where the notation $\bar{\omega} = \frac{1}{|\Omega|} \int_{\Omega} \omega dx$ denotes the mean value of a function ω on Ω . It is easy to verify that the above relations 1), 2), 3), and 4) are simultaneously satisfied with this choice and consequently the properties 1h), 2h) and 3h) are simultaneously true with choice (e).

Replacing the above expression for $L(\mathbf{u}, \varphi, \psi)$ in Scheme (14), we propose the following space approximation of (5): we are looking for $\varphi_h \in H^1(0, T; V_h)$ satisfying:

$$\begin{aligned} \int_{\Omega} \frac{\partial \varphi_h}{\partial t} \psi dx + \epsilon \int_{\Omega} \nabla \varphi_h \cdot \nabla \psi dx + \alpha \int_{\partial \Omega} \varphi_h \psi ds + \frac{1}{2} \int_{\Omega} (\mathbf{u}_h \cdot \nabla \varphi_h)(\psi - \bar{\psi}) dx \\ - \frac{1}{2} \int_{\Omega} (\mathbf{u}_h \cdot \nabla \psi)(\varphi_h - \bar{\varphi}_h) dx = \int_{\Omega} f \psi dx, \quad \forall \psi \in V_h. \end{aligned} \quad (17)$$

Remark 2. As said before, if we want to eliminate some spurious numerical oscillations in dominated convection problem, we add a SUPG term (15) in the numerical scheme (17). We can see that above properties are unchanged with this term.

On a practical point of view, it is not easy to work with Scheme (17) and we can rewrite it on another form. If W is a space of integrable functions defined on Ω , we will denote by $\widetilde{W} = \{g \in W : \int_{\Omega} g dx = 0\}$, and if $\omega \in W$, we will define $\widetilde{\omega} = \omega - \bar{\omega} \in \widetilde{W}$. Let us consider $\widetilde{\varphi}_h \in H^1(0, T; \widetilde{V}_h)$ and $\bar{\varphi}_h \in H^1(0, T; \mathbb{R})$ solution of both equations:

$$\begin{aligned} \int_{\Omega} \frac{\partial \widetilde{\varphi}_h}{\partial t} \psi dx + \epsilon \int_{\Omega} \nabla \widetilde{\varphi}_h \cdot \nabla \psi dx + \alpha \int_{\partial \Omega} (\bar{\varphi}_h + \widetilde{\varphi}_h) \psi ds + \frac{1}{2} \int_{\Omega} (\mathbf{u}_h \cdot \nabla \widetilde{\varphi}_h) \psi dx \\ - \frac{1}{2} \int_{\Omega} (\mathbf{u}_h \cdot \nabla \psi) \widetilde{\varphi}_h dx = \int_{\Omega} f \psi dx, \quad \forall \psi \in \widetilde{V}_h, \end{aligned} \quad (18)$$

and

$$\frac{d}{dt} \int_{\Omega} \bar{\varphi}_h dx + \alpha \int_{\partial \Omega} (\bar{\varphi}_h + \widetilde{\varphi}_h) ds = \int_{\Omega} f dx, \quad (19)$$

with initial condition $\widetilde{\varphi}_h(0) = \varphi_h^0 - \bar{\varphi}_h^0$, where φ_h^0 is an approximation of φ^0 and $\bar{\varphi}_h^0 = \bar{\varphi}_h(0) = \frac{1}{|\Omega|} \int_{\Omega} \varphi_h^0 dx$. We easily verify that by setting $\varphi_h = \widetilde{\varphi}_h + \bar{\varphi}_h$, Problem (17) and Problem (18) – (19) are equivalent.

In (18) the mean value of the test function ψ is vanishing and it is not standard in the finite element method. It is the reason for which this constrain is taken into account by a Lagrange multiplier λ . On the other side we add an equation in order to impose $\int_{\Omega} \tilde{\varphi}_h dx = 0$. Consequently we are looking for $\tilde{\varphi}_h \in H^1(0, T; V_h)$, $\bar{\varphi}_h \in H^1(0, T; \mathbb{R})$ and $\lambda \in H^1(0, T; \mathbb{R})$ satisfying:

$$\begin{aligned} \int_{\Omega} \frac{\partial \tilde{\varphi}_h}{\partial t} \psi dx + \epsilon \int_{\Omega} \nabla \tilde{\varphi}_h \cdot \nabla \psi dx + \alpha \int_{\partial\Omega} (\bar{\varphi}_h + \tilde{\varphi}_h) \psi ds + \frac{1}{2} \int_{\Omega} (\mathbf{u}_h \cdot \nabla \tilde{\varphi}_h) \psi dx \\ - \frac{1}{2} \int_{\Omega} (\mathbf{u}_h \cdot \nabla \psi) \tilde{\varphi}_h dx + \lambda \int_{\Omega} \psi dx = \int_{\Omega} f \psi dx, \quad \forall \psi \in V_h, \end{aligned} \quad (20)$$

$$\frac{d}{dt} \int_{\Omega} \bar{\varphi}_h dx + \alpha \int_{\partial\Omega} (\bar{\varphi}_h + \tilde{\varphi}_h) ds = \int_{\Omega} f dx, \quad (21)$$

$$\int_{\Omega} \tilde{\varphi}_h dx = 0. \quad (22)$$

If the dimension of V_h is N , then (20), (21) and (22) is an ordinary differential system in time with $(N + 2)$ equations where the unknown $\tilde{\varphi}_h$, $\bar{\varphi}$ and λ are coupled. In the case where $\alpha = 0$ (Neumann boundary conditions) the unknown $\bar{\varphi}_h$ is not coupled to the other variables $\tilde{\varphi}_h$ and λ .

3. ERROR ESTIMATES

Now we want to establish error bounds between φ and φ_h in various norms, when φ_h is solution of (17). To do this, we follow [2] and we assume the realistic hypotheses (16) on the velocity field \mathbf{u} and its approximation \mathbf{u}_h .

Let us remark that estimate (16) holds in a lot of standard finite element methods when $\mathbf{u} \in H^2(\Omega)$. In this case \mathbf{u} is continuous on $\bar{\Omega}$. By using the inverse inequality when Γ_h is quasi-regular [1], it follows that there exists a constant C such that

$$\|\mathbf{u} - \mathbf{u}_h\|_{L^\infty(\Omega)} \leq Ch^{1/2}, \quad (23)$$

and consequently $\|\mathbf{u}_h\|_{L^\infty(\Omega)}$ is bounded independently of h . In order to simplify the presentation, we assume in the following that $\mathbf{u}_h \cdot \mathbf{n} = 0$ on the boundary $\partial\Omega$ of Ω , but $\text{div}(\mathbf{u}_h)$ is not necessary vanishing. A consequence of (1) and (16) is that

$$\|\text{div}(\mathbf{u}_h)\| \leq Ch. \quad (24)$$

Robin's boundary conditions

If $\alpha > 0$, then as said above $(\mu, \omega)_1 =_{def} \epsilon \int_{\Omega} \nabla \mu \cdot \nabla \omega dx + \alpha \int_{\partial\Omega} \mu \omega ds$ is a scalar product on $H^1(\Omega)$ equivalent to the standard scalar product on $H^1(\Omega)$. In this case we can define the projector $R_h : \mu \in H^1(\Omega) \rightarrow R_h \mu \in V_h$ by:

$$(\mu - R_h \mu, \omega)_1 = 0, \quad \forall \omega \in V_h, \forall \mu \in H^1(\Omega), \quad (25)$$

and it is well known that if the meshing is regular in the sense of [1], there exists a constant C satisfying

$$\|\mu - R_h\mu\| + h \|\nabla(\mu - R_h\mu)\| \leq Ch^2 \|\mu\|_{H^2(\Omega)} \quad \forall \mu \in H^2(\Omega). \quad (26)$$

In order to prove convergence results, we introduce like in [2] the following notations:

$$\theta = \varphi_h - R_h\varphi \text{ and } \rho = R_h\varphi - \varphi, \quad (27)$$

and we have $\theta + \rho = \varphi_h - \varphi$.

In order to establish some error estimates, we assume that the initial conditions φ^0 and φ_h^0 satisfy

$$\varphi^0 \in H^2(\Omega) \text{ and } \varphi_h^0 = R_h\varphi^0. \quad (28)$$

Lemma 1. *We assume that $\varphi \in C^1([0, T]; H^2(\Omega))$ and that there exists a constant C independent of h such that $\|\varphi_h\|_{L^\infty(\Omega)} \leq C$, $\forall t \in (0, T)$ (L^∞ -stability). Then under Hypothesis (16) there exists a constant \bar{C} independent of h and ϵ which satisfies:*

$$\|\theta(t)\| \leq e^{-\lambda_1 t} \|\theta(0)\| + \int_0^t \|\rho_t(s)\| e^{-\lambda_1(t-s)} ds + \bar{C}ht, \quad 0 < t < T, \quad (29)$$

where $\rho_t = \frac{d}{dt}\rho$.

Proof. By taking $\psi = \theta$ in (5) and (17) we obtain:

$$\begin{aligned} & \int_{\Omega} \frac{\partial}{\partial t} (\varphi - \varphi_h) \theta dx + (\varphi - \varphi_h, \theta)_1 \\ & + \frac{1}{2} \int_{\Omega} ((\theta - \bar{\theta})[\mathbf{u} \cdot \nabla \varphi - \mathbf{u}_h \cdot \nabla \varphi_h] + (\varphi_h - \bar{\varphi}_h) \mathbf{u}_h \cdot \nabla \theta - (\varphi - \bar{\varphi}) \mathbf{u} \cdot \nabla \theta) dx = 0. \end{aligned}$$

In order to evaluate the first term above we write:

$$\begin{aligned} S_1 &= \int_{\Omega} \frac{\partial}{\partial t} (\varphi - \varphi_h) \theta dx \\ &= \int_{\Omega} \frac{\partial}{\partial t} (\varphi - R_h\varphi) \theta dx + \int_{\Omega} \frac{\partial}{\partial t} (R_h\varphi - \varphi_h) \theta dx \\ &= - \int_{\Omega} \rho_t \theta dx - \frac{1}{2} \frac{d}{dt} \|\theta\|^2. \end{aligned}$$

In order to evaluate the second term we use (25) and we write:

$$\begin{aligned} S_2 &= (\varphi - \varphi_h, \theta)_1 \\ &= (\varphi - R_h\varphi, \theta)_1 + (R_h\varphi - \varphi_h, \theta)_1 \\ &= -(\theta, \theta)_1 \leq -\lambda_1 \|\theta\|^2. \end{aligned}$$

It remains to evaluate the third term. Integrating by parts and using (1) with $\mathbf{u}_h \cdot \mathbf{n} = 0$ on $\partial\Omega$, we obtain:

$$\begin{aligned}
S_3 &= \frac{1}{2} \int_{\Omega} ((\theta - \bar{\theta})[\mathbf{u} \cdot \nabla \varphi - \mathbf{u}_h \cdot \nabla \varphi_h] + (\varphi_h - \bar{\varphi}_h) \mathbf{u}_h \cdot \nabla \theta - (\varphi - \bar{\varphi}) \mathbf{u} \cdot \nabla \theta) dx \\
&= \frac{1}{2} \int_{\Omega} (2(\theta - \bar{\theta}) \mathbf{u} \cdot \nabla \varphi - 2(\theta - \bar{\theta}) \mathbf{u}_h \cdot \nabla \varphi_h - (\varphi_h - \bar{\varphi}_h)(\theta - \bar{\theta}) \operatorname{div} \mathbf{u}_h) dx \\
&= \frac{1}{2} \int_{\Omega} (2(\theta - \bar{\theta}) \mathbf{u} \cdot \nabla (\varphi - R_h \varphi) + 2(\theta - \bar{\theta}) \mathbf{u} \cdot \nabla (R_h \varphi - \varphi_h) \\
&\quad + 2(\theta - \bar{\theta})(\mathbf{u} - \mathbf{u}_h) \cdot \nabla \varphi_h - (\theta - \bar{\theta})(\varphi_h - \bar{\varphi}_h) \operatorname{div} \mathbf{u}_h) dx \\
&= \frac{1}{2} \int_{\Omega} (-2(\theta - \bar{\theta}) \mathbf{u} \cdot \nabla \rho - \mathbf{u} \cdot \nabla \theta^2 + 2(\theta - \bar{\theta})(\mathbf{u} - \mathbf{u}_h) \cdot \nabla \varphi_h \\
&\quad - (\theta - \bar{\theta})(\varphi_h - \bar{\varphi}_h) \operatorname{div} \mathbf{u}_h) dx \\
&= \frac{1}{2} \int_{\Omega} (-2(\theta - \bar{\theta}) \mathbf{u} \cdot \nabla \rho + 2(\theta - \bar{\theta})(\mathbf{u} - \mathbf{u}_h) \cdot \nabla \varphi_h - (\theta - \bar{\theta})(\varphi_h - \bar{\varphi}_h) \operatorname{div} \mathbf{u}_h) dx,
\end{aligned}$$

and consequently:

$$|S_3| \leq \left[\|\mathbf{u}\|_{L^\infty(\Omega)} \|\nabla \rho\| + \|\mathbf{u} - \mathbf{u}_h\|_{L^2(\Omega)} \|\nabla \varphi_h\|_{L^\infty(\Omega)} + \frac{1}{2} \|\varphi_h - \bar{\varphi}_h\|_{L^\infty(\Omega)} \|\operatorname{div} \mathbf{u}_h\| \right] \|\theta - \bar{\theta}\|.$$

Taking into account the inverse inequality $\|\nabla \varphi_h\|_{L^\infty(\Omega)} \leq Ch^{-1} \|\varphi_h\|_{L^\infty(\Omega)}$ (see [1]), the inequality $\|\bar{\theta}\| \leq \|\theta\|$ and the fact that $\|\varphi_h\|_{L^\infty(\Omega)}$ is assumed bounded, we obtain with (16) (24):

$$|S_3| \leq C(\|\nabla \rho\| + h) \|\theta\|$$

where here C is a generic constant independent of h and $t \in (0, T)$.

Since we assumed that $\varphi \in C^1([0, T]; H^2(\Omega))$, then by (26), $\|\nabla \rho\|$ is bounded with respect to h and consequently:

$$|S_3| \leq Ch \|\theta\|.$$

Using Estimates S_1 , S_2 , S_3 we finally obtain:

$$\frac{1}{2} \frac{d}{dt} \|\theta\|^2 + \lambda_1 \|\theta\|^2 \leq (\|\rho_t\| + Ch) \|\theta\|,$$

which implies

$$\frac{d}{dt} \|\theta\| + \lambda_1 \|\theta\| \leq (\|\rho_t\| + Ch).$$

Setting $v(t) = \|\theta(t)\| e^{\lambda_1 t}$, we have $\frac{d}{dt} v(t) = (\frac{d}{dt} \|\theta\| + \lambda_1 \|\theta\|) e^{\lambda_1 t} \leq (\|\rho_t\| + Ch) e^{\lambda_1 t}$ and finally:

$$\|\theta(t)\| \leq e^{-\lambda_1 t} \|\theta(0)\| + \int_0^t \|\rho_t(s)\| e^{-\lambda_1(t-s)} ds + \frac{Ch}{\lambda_1} (1 - e^{-\lambda_1 t}).$$

□

Theorem 1. *We assume that $\varphi \in C^1([0, T]; H^2(\Omega))$ and that there exists a constant C independent of h such that $\|\varphi_h\|_{L^\infty(\Omega)} \leq C$, $\forall t \in (0, T)$ (L^∞ -stability). Then under Hypotheses (16) and (28) there exists a constant C_1 independent of h which satisfies:*

$$\|\varphi - \varphi_h\|_{L^\infty(0,T;L^2(\Omega))} \leq C_1 h. \quad (30)$$

Proof. From (26), (28) and Hypothesis $\varphi \in C^1([0, T]; H^2(\Omega))$, we have:

$$\begin{aligned} \|\rho(t)\| &\leq Ch^2 \text{ and } \left(\int_0^t \|\rho_t(s)\|^2 ds\right)^{\frac{1}{2}} \leq Ch^2 \text{ for every } t \in (0, T), \\ \|\theta(0)\| &= \|\varphi_h(0) - \varphi(0)\| \leq Ch^2, \end{aligned}$$

where C is a generic constant. Using Lemma 1 and the equality $\varphi_h - \varphi = \theta + \rho$, we easily prove inequality (30). \square

In order to estimate $\|\nabla(\varphi - \varphi_h)\|_{L^\infty(0,T;L^2(\Omega))}$ we start by proving

Lemma 2. *We assume the hypothesis of Lemma 1. Then there exists a constant C which satisfies*

$$\|\theta_t\|^2 + \frac{1}{2} \frac{d}{dt} \|\theta\|_1^2 \leq \|\theta_t\| [\|\rho_t\| + C(h + \|\theta\|_1)]. \quad (31)$$

where $\theta_t = \frac{d}{dt}\theta$, $\rho_t = \frac{d}{dt}\rho$.

Proof. By taking $\psi = \theta_t$ in (5) and (17) we obtain:

$$\begin{aligned} &\int_{\Omega} \frac{\partial}{\partial t} (\varphi - \varphi_h) \theta_t dx + (\varphi - \varphi_h, \theta_t)_1 \\ &+ \frac{1}{2} \int_{\Omega} (\theta_t - \bar{\theta}_t) [\mathbf{u} \cdot \nabla \varphi - \mathbf{u}_h \cdot \nabla \varphi_h] + (\varphi_h - \bar{\varphi}_h) \mathbf{u}_h \cdot \nabla \theta_t - (\varphi - \bar{\varphi}) \mathbf{u} \cdot \nabla \theta_t dx = 0. \end{aligned}$$

In order to evaluate the first term above we write:

$$\begin{aligned} S_1 &= \int_{\Omega} \frac{\partial}{\partial t} (\varphi - \varphi_h) \theta_t dx \\ &= \int_{\Omega} \frac{\partial}{\partial t} (\varphi - R_h \varphi) \theta_t dx + \int_{\Omega} \frac{\partial}{\partial t} (R_h \varphi - \varphi_h) \theta_t dx \\ &= - \int_{\Omega} \rho_t \theta_t dx - \|\theta_t\|^2. \end{aligned}$$

In order to evaluate the second term we write:

$$\begin{aligned} S_2 &= (\varphi - \varphi_h, \theta_t)_1 \\ &= (R_h \varphi - \varphi_h, \theta_t)_1 - \frac{1}{2} \frac{d}{dt} \|\theta\|_1^2. \end{aligned}$$

The third term is evaluated like in Lemma 1:

$$\begin{aligned}
S_3 &= \frac{1}{2} \int_{\Omega} ((\theta_t - \bar{\theta}_t)[\mathbf{u} \cdot \nabla \varphi - \mathbf{u}_h \cdot \nabla \varphi_h] + (\varphi_h - \bar{\varphi}_h) \mathbf{u}_h \cdot \nabla \theta_t - (\varphi - \bar{\varphi}) \mathbf{u} \cdot \nabla \theta_t) dx \\
&= \frac{1}{2} \int_{\Omega} (2(\theta_t - \bar{\theta}_t) \mathbf{u} \cdot \nabla \varphi - 2(\theta_t - \bar{\theta}_t) \mathbf{u}_h \cdot \nabla \varphi_h - (\varphi_h - \bar{\varphi}_h)(\theta_t - \bar{\theta}_t) \operatorname{div} \mathbf{u}_h) dx \\
&= \frac{1}{2} \int_{\Omega} (-2(\theta_t - \bar{\theta}_t) \mathbf{u} \cdot \nabla \rho - 2(\theta_t - \bar{\theta}_t) \mathbf{u} \cdot \nabla \theta \\
&\quad + 2(\theta_t - \bar{\theta}_t)(\mathbf{u} - \mathbf{u}_h) \cdot \nabla \varphi_h - (\varphi_h - \bar{\varphi}_h)(\theta_t - \bar{\theta}_t) \operatorname{div} \mathbf{u}_h) dx.
\end{aligned}$$

It follows with $\|\nabla \rho\| \leq Ch$ (see (26)) and $\|\nabla \theta\|^2 \leq \frac{1}{\epsilon} \|\theta\|_1^2$ that:

$$|S_3| \leq \left[\|\mathbf{u}\|_{L^\infty(\Omega)} C(h + \|\theta\|_1) + \|\mathbf{u} - \mathbf{u}_h\| \|\nabla \varphi_h\|_{L^\infty(\Omega)} + \frac{1}{2} \|\operatorname{div} \mathbf{u}_h\| \|(\varphi_h - \bar{\varphi}_h)\|_{L^\infty(\Omega)} \right] \|(\theta_t - \bar{\theta}_t)\|$$

and with (16), (23), and the inverse inequality $\|\nabla \varphi_h\|_{L^\infty(\Omega)} \leq Ch^{-1} \|\varphi_h\|_{L^\infty(\Omega)}$, we obtain $|S_3| \leq C(h + \|\theta\|_1) \|\theta_t\|$ and finally the announced result of Lemma 2. \square

Theorem 2. *We assume that $\varphi \in C^1([0, T]; H^2(\Omega))$ and that there exists a constant C independent of h such that $\|\varphi_h\|_{L^\infty(\Omega)} \leq C$, $\forall t \in (0, T)$ (L^∞ -stability). Then under Hypotheses (16) and (28) there exists a constant C_2 independent of h which satisfies:*

$$\|\varphi - \varphi_h\|_{L^\infty(0, T; H^1(\Omega))} \leq C_2 h. \quad (32)$$

Proof. We have

$$\begin{aligned}
\|\theta_t\| [\|\rho_t\| + C(h + \|\theta\|_1)] &\leq \frac{1}{2} \|\theta_t\|^2 + \frac{1}{2} [\|\rho_t\| + C(h + \|\theta\|_1)]^2 \\
&\leq \frac{1}{2} \|\theta_t\|^2 + \|\rho_t\|^2 + 2C^2(h^2 + \|\theta\|_1^2).
\end{aligned}$$

The inequality of Lemma 2 implies if C is a generic constant:

$$\frac{1}{2} \|\theta_t\|^2 + \frac{1}{2} \frac{d}{dt} \|\theta\|_1^2 \leq C(h^2 + \|\theta\|_1^2) + \|\rho_t\|^2.$$

From this above relation we obtain $\|\theta(t)\|_1^2 \leq C(\|\theta(0)\|_1^2 + h^2 + \int_0^t \|\rho_t(s)\|^2 ds)$.

Since $\varphi \in C^1([0, T]; H^2(\Omega))$, there exists a constant C such that:

$$\|\theta(t)\|_1^2 \leq C(\|\theta(0)\|_1^2 + h^2) \text{ for every } t \in (0, T).$$

Relations (26) and (28) imply that $\|\theta(0)\|_1 \leq Ch$. Finally by (26) : $\|\varphi - \varphi_h\|_1 = \|\theta + \rho\|_1 \leq Ch$ for every $t \in [0, T]$. \square

Neumann boundary conditions

If $\alpha = 0$ then $(\mu, \omega)_1 =_{def} \epsilon \int_{\Omega} \nabla \mu \cdot \nabla \omega dx$ is a scalar product on $\tilde{H}^1(\Omega)$. In this case we can define the operator $R_h : \mu \in \tilde{H}^1(\Omega) \rightarrow R_h \mu \in \tilde{V}_h$ by:

$$(\mu - R_h \mu, \omega)_1 = 0, \quad \forall \omega \in \tilde{V}_h, \forall \mu \in \tilde{H}^1(\Omega), \quad (33)$$

and in this case $\lambda_1 = \inf_{\mu \in \tilde{H}^1(\Omega)} \frac{(\mu, \mu)_1}{\|\mu\|^2}$. Moreover we have seen that if we decompose φ and φ_h by $\varphi = \bar{\varphi} + \tilde{\varphi}$ and $\varphi_h = \bar{\varphi}_h + \tilde{\varphi}_h$, then the equations for $\tilde{\varphi}$ and $\bar{\varphi}$ are not coupled and analogously for $\tilde{\varphi}_h$ and $\bar{\varphi}_h$. By defining $\theta = \tilde{\varphi}_h - R_h \tilde{\varphi}$ and $\rho = R_h \tilde{\varphi} - \tilde{\varphi}$, then Lemma 1 and 2 remains true (see [11]) for functions with zero meanvalue and allow to obtain Theorem 1 and 2 even if $\alpha = 0$.

4. DISCRETIZATION IN TIME WITH A CONSERVATIVE SCHEME

In this section we treat only the case $\alpha > 0$. Let us consider a backward Euler scheme in order to discretize (17) in time. If $0 = t_0 < t_1 < t_2 < \dots < t_n < \dots < t_N = T$ is a discretization of the time interval $[0, T]$ and if we assume that we know the approximations $\varphi_h^n \simeq \varphi_h(t_n)$ at time t_n , we are looking for $\varphi_h^{n+1} \in V_h$ satisfying

$$\begin{aligned} \int_{\Omega} \frac{\varphi_h^{n+1} - \varphi_h^n}{t_{n+1} - t_n} \psi dx + \epsilon \int_{\Omega} \nabla \varphi_h^{n+1} \cdot \nabla \psi dx + \alpha \int_{\partial \Omega} \varphi_h^{n+1} \psi ds \\ + \frac{1}{2} \int_{\Omega} (\mathbf{u}_h \cdot \nabla \varphi_h^{n+1}) (\psi - \bar{\psi}) dx - \frac{1}{2} \int_{\Omega} (\mathbf{u}_h \cdot \nabla \psi) (\varphi_h^{n+1} - \bar{\varphi}_h^{n+1}) dx \\ = \int_{\Omega} f(t^{n+1}) \psi dx, \quad \forall \psi \in V_h. \end{aligned} \quad (34)$$

Remark 3. In practice, for solving Problem (34) with the finite element method we decompose $\varphi_h^{n+1} = \bar{\varphi}_h^{n+1} + \tilde{\varphi}_h^{n+1}$ and we introduce a Lagrange multiplier in order to take into account that $(\psi - \bar{\psi})$ is zero meanvalue as in (20), (21), (22).

Remark 4. When we take $\psi = \varphi_h^{n+1}$ in (34) we obtain:

$$\|\varphi_h^{n+1}\|^2 + (t_{n+1} - t_n) \|\varphi_h^{n+1}\|_1^2 \leq \int_{\Omega} \varphi_h^{n+1} \varphi_h^n dx + (t_{n+1} - t_n) \|f(t^{n+1})\| \|\varphi_h^{n+1}\|$$

and it follows

$$(1 + \lambda_1 (t_{n+1} - t_n)) \|\varphi_h^{n+1}\| \leq \|\varphi_h^n\| + (t_{n+1} - t_n) \|f(t^{n+1})\|. \quad (35)$$

Properties (1h), (2h), (3h) mentioned in Section 1 are satisfied with the scheme (34).

In order to establish an error estimate we proceed again like in [2]. We limit us to the case $\alpha > 0$ and we set analogously to (27)

$$\theta^n = \varphi_h^n - R_h \varphi(t_n) \quad \text{and} \quad \rho^n = R_h \varphi(t_n) - \varphi(t_n). \quad (36)$$

In order to simplify the notations, we denote by

$$r_{n+1} = t_{n+1} - t_n \text{ and } \varphi^n = \varphi(t_n), \quad (37)$$

$$\bar{\partial}\theta^{n+1} = (\theta^{n+1} - \theta^n) / (t_{n+1} - t_n) \quad (38)$$

$$\tau = \max_{1 \leq n \leq N} r_n. \quad (39)$$

Theorem 3. *We assume that $\varphi \in C^1([0, T]; H^2(\Omega)) \cap C^2([0, T]; L^2(\Omega))$ and that there exists a constant C independent of h and n such that $\|\varphi_h^n\|_{L^\infty(\Omega)} \leq C$, (L^∞ - stability). Then under Hypotheses (16) and (28), there exists a constant C_3 independent of h which satisfies:*

$$\|\varphi(t_n) - \varphi_h^n\|_{L^2(\Omega)} \leq C_3(h + \tau) \text{ for every } 0 < n \leq N. \quad (40)$$

Proof. The proof of Theorem 3 is very similar to the proof of Theorem 1 via Lemma 1. By choosing $\psi = \theta^{n+1}$ in (5) and in (34), we obtain with an integration by parts of the term $\frac{1}{2} \int_{\Omega} (\mathbf{u}_h \cdot \nabla \psi) \varphi_h^{n+1} dx$:

$$\int_{\Omega} \bar{\partial}\theta^{n+1} \cdot \theta^{n+1} dx + \|\theta^{n+1}\|_1^2 = \int_{\Omega} (\omega_1^{n+1} + \omega_2^{n+1}) \theta^{n+1} dx \quad (41)$$

with

$$\omega_1^{n+1} = \mathbf{u} \cdot \nabla \varphi^{n+1} - \mathbf{u}_h \cdot \nabla \varphi_h^{n+1} - \frac{1}{2} \operatorname{div}(\mathbf{u}_h) (\varphi_h^{n+1} - \bar{\varphi}_h^{n+1})$$

and

$$\omega_2^{n+1} = \frac{\partial \varphi}{\partial t}(t_{n+1}) - \bar{\partial} R_h \varphi^{n+1}.$$

Error estimate of $\int_{\Omega} \omega_1^{n+1} \theta^{n+1} dx$ is made as S_3 in Lemma 1 by replacing θ by θ^{n+1} , i.e.

$$\left| \int_{\Omega} \omega_1^{n+1} \cdot \theta^{n+1} dx \right| \leq C(\|\nabla \rho^{n+1}\| + h) \|\theta^{n+1}\| \leq Dh \|\theta^{n+1}\|, \quad (42)$$

where C, D are two constants independent of h and n . Error estimate of $\int_{\Omega} \omega_2^{n+1} \theta^{n+1} dx$ follows from (26):

$$\left| \int_{\Omega} \omega_2^{n+1} \theta^{n+1} dx \right| \leq \left| \int_{\Omega} \left(\frac{\partial \varphi}{\partial t}(t_{n+1}) - \bar{\partial} \varphi^{n+1} \right) \theta^{n+1} dx \right| + \left| \int_{\Omega} \bar{\partial} \rho^{n+1} \theta^{n+1} dx \right|$$

and consequently, since we have assumed $\varphi \in C^1([0, T]; H^2(\Omega)) \cap C^2([0, T]; L^2(\Omega))$:

$$\left| \int_{\Omega} \omega_2^{n+1} \theta^{n+1} dx \right| \leq C(r_{n+1} + r_{n+1} h^2) \|\theta^{n+1}\| \leq D\tau \|\theta^{n+1}\|. \quad (43)$$

From (41), (42) and (43) we obtain:

$$\|\theta^{n+1}\| \leq [\|\theta^n\| + Cr_{n+1}(\tau + h)].$$

Taking into account that $\sum_{j=1}^n r_j = t_n$, we finally obtain:

$$\|\theta^n\| \leq \|\theta^0\| + Ct_n(\tau + h) \leq \|\theta^0\| + CT(\tau + h).$$

In order to complete the proof of Theorem 3, we use the same arguments that we gave in the proof of Theorem 1. \square

By choosing $\psi = \bar{\partial}\theta^{n+1}$ in (5) and in (34), like in Theorems 2 and 3, it is standard to prove the following result (see [2] and [10]):

Theorem 4. *We assume the hypotheses of Theorem 3. Then there exists a constant C_4 such that*

$$\|\nabla(\varphi(t_n) - \varphi_h^n)\|_{L^2(\Omega)} \leq C_4(h + \tau) \quad \text{for every } 0 < n \leq N. \quad (44)$$

5. NUMERICAL RESULTS

We now check numerically that the conservative scheme developed in this article has the desired properties, even if we have stabilisation terms. Let Ω be the domain $[-1, 1]^2 \times [-0.1, 0.1]$ and

$$\mathbf{u}(x, y, z) = \left(-\cos\left(\frac{3\pi x}{2}\right)\sin\left(\frac{3\pi y}{2}\right), \sin\left(\frac{3\pi x}{2}\right)\cos\left(\frac{3\pi y}{2}\right), 0\right). \quad (45)$$

It is easy to remark that $\mathbf{u} \cdot \mathbf{n} = 0$ on $\partial\Omega$ and that $\operatorname{div} \mathbf{u} = 0$. We also define the following exchange coefficient

$$\alpha = \begin{cases} 1 & \text{if } |z| < 0.1 \\ 0 & \text{if } |z| = 0.1 \end{cases}$$

which means that the domain is isolated on its top and bottom and in this particular case, the phenomenon are two-dimensional. Setting $\epsilon = 10^{-5}$, we numerically solve the following problem : find $\varphi : (0, T) \times \Omega \rightarrow \mathbb{R}$ such that

$$\begin{cases} \frac{\partial \varphi}{\partial t} - \epsilon \Delta \varphi + \mathbf{u} \cdot \nabla \varphi = f & \text{in } \Omega \\ \epsilon \frac{\partial \varphi}{\partial \mathbf{n}} = -\alpha \varphi & \text{on } \partial\Omega \\ \varphi(0) = \varphi_0. \end{cases} \quad (46)$$

Let \mathcal{T}_h be a uniform discretisation of the domain Ω with parameter $h = 0.1$, $\Delta t = T/N$, $t_n = n\Delta t$, $n = 0, \dots, N$ and V_h the space of piecewise linear finite elements. The space-time discretisation using backward Euler method of (46) becomes : given $\varphi_h^0 = \varphi_0$, for $n = 0, \dots, N-1$, we are looking for $\varphi_h^{n+1} \in V_h$ satisfying

$$\begin{cases} \int_{\Omega} \frac{\varphi_h^{n+1} - \varphi_h^n}{\Delta t} \psi_h dx + \int_{\Omega} \epsilon \nabla \varphi_h^{n+1} \cdot \nabla \psi_h dx + \int_{\Omega} L(\mathbf{u}_h, \varphi_h^{n+1}, \psi_h) dx \\ \quad + \int_{\partial\Omega} \alpha \varphi_h^{n+1} \psi_h ds + \sum_{K \in \mathcal{T}_h} \int_K \beta_1 \delta_K \frac{h_K}{\|\mathbf{u}_h\|} (\mathbf{u}_h \cdot \nabla \varphi_h^{n+1})(\mathbf{u}_h \cdot \nabla \psi_h) dx \\ \quad + \sum_{K \in \mathcal{T}_h} \int_K \beta_2 \delta_K h_K \|\mathbf{u}_h\| (\nabla \varphi_h^{n+1} \cdot \nabla \psi_h) dx = \int_{\Omega} f^{n+1} \psi_h dx \end{cases} \quad (47)$$

for all $\psi_h \in V_h$, where β_1 is a stabilisation parameter, β_2 an artificial diffusion parameter, δ_K is a function of local Péclet number $\mathbb{P}e_K$, i.e. $\delta_K = 1$ if $\mathbb{P}e_K \geq 1$ and $\delta_K = \mathbb{P}e_K$ if not. In (47), $L(\mathbf{u}_h, \varphi_h^{n+1}, \psi_h)$ is a discretisation of the convective term, where \mathbf{u}_h is an approximation of the velocity field (45). In our computation, \mathbf{u}_h is obtained using a $\mathbb{P}_1 - \mathbb{P}_1$ stabilized stationary Navier-Stokes solver in which the force term is such that (45) is a solution of the Navier-Stokes equations with pressure $p(x, y, z) = \frac{1}{4}(\cos(3\pi x) + \cos(3\pi y))$. The velocity field \mathbf{u}_h is computed only once, before solving (46), and then used for every computation of φ_h^{n+1} .

In (47), we added a SUPG stabilization term and an artificial diffusion term, because $h_K > \epsilon/\|\mathbf{u}\|_{L^2(K)}$. These stabilisation terms do not influence energy conservation, because both terms vanish when the test function $\psi_h \equiv 1$ is taken. Nevertheless we have to take them into account for L^2 stability verification, because they do not vanish when $\psi_h \equiv \varphi_h^{n+1}$ but both are positive and contribute to stabilize the scheme.

We just describe here the properties that we claim our scheme is numerically conserving. The first one is the energy conservation, which states that

$$\frac{d}{dt} \int_{\Omega} \varphi dx = \int_{\Omega} f dx + \int_{\partial\Omega} \alpha(\varphi_r - \varphi) ds.$$

In our numerical tests, $\varphi_r \equiv 0$ and using backward Euler for time discretisation of (10), we obtain the discrete energy conservation : for $n = 0, \dots, N-1$

$$\int_{\Omega} \varphi_h^{n+1} dx + \int_{\partial\Omega} \alpha \varphi_h^{n+1} ds = \int_{\Omega} \varphi_h^n + \Delta t \int_{\Omega} f^{n+1} dx \quad (48)$$

Proceeding the same manner as above, and taking into account the stabilisation terms, we can deduce that the discrete L^2 stability property is : for $n = 0, \dots, N-1$

$$\begin{aligned} \|\varphi_h^{n+1}\|_{L^2(\Omega)}^2 + \Delta t \left(\int_{\partial\Omega} \alpha (\varphi_h^{n+1})^2 ds + \int_{\Omega} \epsilon |\nabla \varphi_h^{n+1}|^2 dx \right) + \Delta t (S_1(\varphi_h^{n+1}, \varphi_h^{n+1}) + S_2(\varphi_h^{n+1}, \varphi_h^{n+1})) \\ = \int_{\Omega} \varphi_h^{n+1} \varphi_h^n dx + \Delta t \int_{\Omega} f^{n+1} \varphi_h^{n+1} dx \end{aligned} \quad (49)$$

where

$$S_1(\varphi_h, \psi_h) = \sum_{K \in \mathcal{T}_h} \int_K \beta_1 \delta_K \frac{h_K}{\|\mathbf{u}_h\|} (\mathbf{u}_h \cdot \nabla \varphi_h) (\mathbf{u}_h \cdot \nabla \psi_h) dx$$

and

$$S_2(\varphi_h, \psi_h) = \sum_{K \in \mathcal{T}_h} \int_K \beta_2 \delta_K h_K \|\mathbf{u}_h\| (\nabla \varphi_h \cdot \nabla \psi_h) dx.$$

Remark that $S_1(\varphi_h, \varphi_h)$ and $S_2(\varphi_h, \varphi_h)$ are positive and contribute to the L^2 -stability. Finally, the third one is the conservation of constant solution.

We now focus on the discretisation of the convective term $L(\mathbf{u}_h, \varphi_h, \psi_h)$. We recall that they are mainly four standard possibilities if we do not use the scheme proposed in this paper

- L1. $L(\mathbf{u}_h, \varphi_h, \psi_h) = (\mathbf{u}_h \cdot \nabla \varphi_h) \psi_h$,
- L2. $L(\mathbf{u}_h, \varphi_h, \psi_h) = -(\mathbf{u}_h \cdot \nabla \psi_h) \varphi_h$,
- L3. $L(\mathbf{u}_h, \varphi_h, \psi_h) = \text{div}(\mathbf{u}_h \varphi_h) \psi_h$,
- L4. $L(\mathbf{u}_h, \varphi_h, \psi_h) = \frac{1}{2}(\mathbf{u}_h \cdot \nabla \varphi_h) \psi_h - \frac{1}{2}(\mathbf{u}_h \cdot \nabla \psi_h) \varphi_h$,

and our scheme is to take

$$\text{L5. } L(\mathbf{u}_h, \varphi_h, \psi_h) = \frac{1}{2}(\mathbf{u}_h \cdot \nabla \varphi_h)(\psi_h - \bar{\psi}_h) - \frac{1}{2}(\mathbf{u}_h \cdot \nabla \psi_h)(\varphi_h - \bar{\varphi}_h)$$

Due to the fact that $\text{div } \mathbf{u}_h$ is not equal to zero, each of the first four discretisations conserves in principle and a priori only one of the three desired properties. Of course, scheme L5 is the only one which conserves the three properties. The Table 1 summarizes the properties of each $L(\mathbf{u}_h, \varphi_h, \psi_h)$.

$L(\mathbf{u}_h, \varphi_h, \psi_h)$	Energy conservation	L^2 stability	Const. sol. conservation
L1	no	no	yes
L2	yes	no	no
L3	yes	no	no
L4	no	yes	no
L5	yes	yes	yes

TABLE 1. Properties conserved by different discretisations of convective term.

We could notice in Table 1 that only one property is conserved for each discretisation, except for the scheme developed in this article.

To check the conservation of energy and L^2 -stability, we compute f in (46) in such a way the solution φ is given by

$$\varphi(t, x, y, z) = (1 - e^{-\lambda t}) \left[\frac{\cos(x) - \cos(1)}{\epsilon} + \sin(1) \right] \left[\frac{\cos(y) - \cos(1)}{\epsilon} + \sin(1) \right]$$

with $\lambda = 0.005$. It is with this right hand member f that we will compute φ_h^{n+1} solution of (47) with α and ϵ defined as before. For numerical approximation, we use $\Delta t = 1$ and made 3000 iterations. At each time step n , we compute the quantity

$$\Delta P1(n) = \frac{|I_1 - I_2|}{|I_1|}$$

where I_1, I_2 are respectively the left hand side and right hand side of (48). We can notice that if the energy conservation property is satisfied, $\Delta P1(n) = 0$ for $n = 0, \dots, N - 1$. Similarly, for L^2 stability, we compute at each time step the estimator

$$\Delta P2(n) = \frac{|J_1 - J_2|}{|J_1|} \quad (50)$$

where J_1, J_2 are respectively the left hand side and right hand side of (49). As above, $\Delta P2(n) = 0$ if and only if the discrete L^2 stability is achieved.

Let $\varphi_r \equiv 10$, ϵ , α and \mathbf{u} as before. To verify the conservation of constant solution, we solve the following problem

$$\begin{cases} \frac{\partial \varphi}{\partial t} - \epsilon \Delta \varphi + \mathbf{u} \cdot \nabla \varphi = 0 & \text{in } \Omega \\ \epsilon \frac{\partial \varphi}{\partial \mathbf{n}} = \alpha(\varphi_r - \varphi) & \text{on } \partial \Omega \\ \varphi(0) = \varphi_r, \end{cases} \quad (51)$$

and the solution is $\varphi \equiv \varphi_r$ for every t . Of course, we adapt numerical scheme (47) to problem (51) by adding $\int_{\partial \Omega} \varphi_r \psi_h dx$ to the right hand side of (47). The estimator that we use to check the conservation of constant solution at each time step $n = 0, \dots, N - 1$ is

$$\Delta P3(n) = \frac{\|\varphi_r - \varphi_h^{n+1}\|_{L^\infty}}{\|\varphi_r\|_{L^\infty}}. \quad (52)$$

Defining

- $\Pi_1 = \max_{0 \leq n \leq N-1} \Delta P1(n)$,
- $\Pi_2 = \max_{0 \leq n \leq N-1} \Delta P2(n)$,
- $\Pi_3 = \max_{0 \leq n \leq N-1} \Delta P3(n)$,

we obtained the results shown in table 2.

$L(\mathbf{u}_h, \varphi_h, \psi_h)$	Π_1	Π_2	Π_3
L1	$1.56 \cdot 10^{-4}$	0.0015	$1.50 \cdot 10^{-10}$
L2	$4.17 \cdot 10^{-11}$	0.0014	0.0035
L3	$4.02 \cdot 10^{-11}$	0.0015	0.0035
L4	$8.48 \cdot 10^{-5}$	$1.21 \cdot 10^{-12}$	0.0018
L5	$1.14 \cdot 10^{-11}$	$3.38 \cdot 10^{-12}$	$7.11 \cdot 10^{-14}$

TABLE 2. Numerical verification of the properties 1 to 3.

The results of Table 2 exactly match what we claimed on Table 1. We can also notice that numerical scheme L5 is the only one which numerically satisfies the three conservation properties.

6. CONCLUSION

In order to conclude this presentation, we claim that only the numerical scheme corresponding to L5 is efficient in the application when we numerically treat the coupling incompressible Navier-Stokes equations with the convection-diffusion equation, as in [12] and [13]

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