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## A combined finite volume– nonconforming/mixed-hybrid finite element scheme for degenerate parabolic problems

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**Abstract** We propose and analyze a numerical scheme for nonlinear degenerate parabolic convection-diffusion-reaction equations in two or three space dimensions. We discretize the diffusion term, which generally involves an inhomogeneous and anisotropic diffusion tensor, over an unstructured simplicial mesh of the space domain by means of the piecewise linear nonconforming (Crouzeix-Raviart) finite element method, or using the stiffness matrix of the hybridization of the lowest-order Raviart–Thomas mixed finite element method. The other terms are discretized by means of a cell-centered finite volume scheme on a dual mesh, where the dual volumes are constructed around the sides of the original mesh. Checking the local Péclet number, we set up the exact necessary amount of upstream weighting to avoid spurious oscillations in the convection-dominated case. This technique also ensures the validity of the discrete maximum principle under some conditions on the mesh and the diffusion tensor. We prove the convergence

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M. Vohralík Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 120 00 Prague 2, Czech Republic. E-mail: vohralik@km1.fjfi.cvut.cz of the scheme, only supposing the shape regularity condition for the original mesh. We use a priori estimates and the Kolmogorov relative compactness theorem for this purpose. The proposed scheme is robust, only 5-point (7-point in space dimension three), locally conservative, efficient, and stable, which is confirmed by numerical experiments.

**Keywords** nonlinear degenerate parabolic convection–diffusion–reaction equation  $\cdot$  anisotropic diffusion tensor  $\cdot$  finite volume method  $\cdot$  nonconforming finite element method  $\cdot$  convergence of approximate solutions

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## **1** Introduction

Degenerate parabolic equations arise in many contexts, such as flow in porous media or free boundary problems. This paper is motivated by the modeling of contaminant transport in porous media with equilibrium adsorption reaction, see [7, 10], that typically involves a convection–diffusion–reaction equation of the form

$$\frac{\partial \beta(c)}{\partial t} - \nabla \cdot (\mathbf{S} \nabla c) + \nabla \cdot (c \mathbf{v}) + F(c) = q, \qquad (1.1)$$

where *c* is the unknown concentration of the contaminant, the function  $\beta(\cdot)$  represents time evolution and equilibrium adsorption reaction and is supposed to be continuous and increasing with the growth bounded from below by a positive constant, **S** is the diffusion–dispersion tensor, **v** is the velocity field in the convection term (given for instance by the Darcy law), the function  $F(\cdot)$  represents the changes due to chemical reactions, and finally, *q* stands for the sources. Equation (1.1) is degenerate parabolic since  $\beta'$  may be unbounded, generally dominated by the convection term, and involves inhomogeneous and anisotropic (nonconstant full-matrix) diffusion–dispersion tensor.

A large variety of methods have been proposed for the discretization of degenerate parabolic equations. The conforming piecewise linear finite element method has been studied e.g. by Barrett and Knabner [8], Chen and Ewing [15], Ebmeyer [22], Nochetto *et al* [37], and Rulla and Walkington [40], the cell-centered finite volume method by Baughman and Walkington [9] and Eymard *et al* [25, 26], the vertex-centered finite volume method by Ohlberger [38], the finite difference method e.g. by Karlsen *et al* [35], the mixed finite element method by Arbogast *et al* [4] or Dawson [19], characteristic or Eulerian–Lagrangian methods e.g. by Jäger and Kačur [33]. We shall follow in this paper the finite element/finite volume approach.

The finite element method allows for an easy discretization of the diffusion term with a full tensor and does not impose any restrictions on the meshes. However, it is well-known that numerical instabilities may arise in the convectiondominated case. Recall that contrary to a widely held opinion, this method is locally conservative, cf. Forsyth [31], Eymard *et al* [23, Section III.12], or a detailed analysis given in Hughes *et al* [32]. The cell-centered finite volume method with an upwind discretization of the convection term ensures the stability and is extremely robust and computationally inexpensive. However, the mesh for the discretization of the diffusion term has to fulfill the following orthogonality property: the line segment relying the emplacement of the unknowns in two neighboring volumes has to be orthogonal to the side (edge in space dimension two and face in space dimension three) between these volumes, cf. [23]. Also, there is no straightforward way to apply this finite volume method to problems with full diffusion tensors. Various "multi-point" schemes where the approximation of the flux through an edge involves several scalar unknowns have been proposed, cf. e.g. Aavatsmark *et al* [1], Coudière *et al* [18], Eymard *et al* [24], or Faille [29]. However, such schemes require using more points than the classical 4 points for triangular meshes and 5 points for quadrangular meshes in space dimension two, making the schemes less robust. Their extension to three-dimensional unstructured meshes is also not straightforward (with the exception of the scheme proposed in [24]).

A quite intuitive idea is hence to combine a finite element discretization of the diffusion term with a finite volume discretization of the other terms of (1.1), trying to use the "best of both worlds". Schemes combining conforming piecewise linear finite elements on triangles for the diffusion term with  $\mathbf{S} = Id$  and finite volumes on dual volumes associated with the vertices, proposed and studied by Debiez *et al* [20] or Feistauer *et al* [30] for fluid mechanics equations, are indeed quite efficient. Our motivation is to extend these ideas to degenerate parabolic problems, to the combination of the mixed-hybrid finite element and finite volume methods, to inhomogeneous and anisotropic diffusion–dispersion tensors, to space dimension three, and finally to meshes only satisfying the shape regularity condition.

Let us now introduce the combined scheme that we analyze in this paper. We consider a triangulation of the space domain consisting of simplices (triangles in space dimension two and tetrahedra in space dimension three). We next construct a dual mesh where the dual volumes are associated with the sides (edges or faces). To construct a dual volume, one connects the barycentres of two neighboring simplices through the vertices of their common side. We finally place the unknowns in the barycentres of the sides. For the discretization of the diffusion term of (1.1), we consider the piecewise linear nonconforming (Crouzeix-Raviart) finite element method or the mixed-hybrid finite element method where the only unknowns are the Lagrange multipliers, cf. Arnold and Brezzi [5], Brezzi and Fortin [12]. We recall that although obtained on a basis of completely different considerations (minimization of a quadratic functional over a nonconforming finite element space in the first case, easier implementation of the mixed finite element method in the second case), the elements of the obtained stiffness matrices have to naturally express the coefficients for the discrete diffusive fluxes between the unknowns. Hence, to obtain the combined scheme, we perform a finite volume discretization of (1.1)over the dual mesh and consequently replace the finite volume stiffness matrix corresponding to the diffusion term by one of the above finite element stiffness matrices. The combination of finite volumes with nonconforming finite elements was originally proposed and analyzed by Angot *et al* [3] as a semi-implicit discretization of a convection-diffusion equation with a nonlinear convection term in space dimension two. As far as we know, the combination of the finite volume method with the mixed-hybrid method is new. However, the two finite element stiffness matrices are very close. For a piecewise constant diffusion tensor, they

completely coincide (see Arnold and Brezzi [5] and Chen [14]), and for a general diffusion tensor, the stiffness matrix of the mixed-hybrid method is the stiffness matrix of the nonconforming method with a piecewise constant diffusion tensor, given as the elementwise harmonic average of the original one (see Lemma 8.1 and Remark 3.2 below).

We propose the combined scheme for the equation (1.1) in combination with the backward Euler finite difference time stepping. We can mention its following advantages. The scheme inherits the diffusion properties of nonconforming/mixed-hybrid finite elements, enabling in particular the use of general meshes and the discretization of anisotropic diffusion tensors. It next possesses the discrete maximum principle in the case where all transmissibilities are non-negative. This happens for instance when the diffusion tensor reduces to a scalar function and when the angles between the outward normal vectors of sides of each simplex in the triangulation are greater or equal to  $\pi/2$ . Moreover, we achieve this stability by checking the local Péclet number and by adding side-by-side the exact necessary amount of upstream weighting in order to reduce the excessive smearing of the full upwinding but to still guarantee the discrete maximum principle. The scheme is numerically still stable even in the case where there exist negative transmissibilities, although the discrete maximum principle is no more guaranteed. The undershoots and overshoots only come in this case from the diffusion term, since we avoid the spurious oscillations in the convection-dominated regime by changing the numerical flux to the full upwind one. The scheme is next locally conservative in the sense that the sum of the fluxes over the sides of each (dual) cell equals the time-accumulation, sources, and reaction term in this cell and that the (both diffusive and convective) fluxes are continuous across each (dual) side. It is only 5-point in space dimension two and 7-point in space dimension three. It finally permits to efficiently discretize degenerate parabolic problems: when we search for the discrete unknowns corresponding to  $\beta(c)$ , the resulting system of nonlinear algebraic equations can be solved by the Newton method without any parabolic regularization (cf. Barrett and Knabner [8]) or perturbation of initial and boundary conditions (cf. Pop and Yong [39]), which make the equation uniformly parabolic. Moreover, the resulting matrices are diagonal for the part of the unknowns which correspond to the region where the approximate solution is equal to zero.

Our numerical scheme permits to construct approximate solutions that are piecewise constant on the dual mesh or piecewise linear on the primal simplicial mesh and continuous in the barycentres of the sides of the simplices. We prove the convergence of both these approximations to a weak solution of the continuous problem in this paper. The methods of proof are based upon the Kolmogorov relative compactness theorem and the finite volume tools from [23]. We extend these tools onto schemes with negative transmissibilities, for cases where the discrete maximum principle is not satisfied, and for (dual) meshes not necessarily satisfying the orthogonality property. We only need the shape regularity (minimal angle) assumption for the primal triangulation, we require neither the inverse assumption (bounded ratio between the diameters of elements in the primal mesh), nor any maximal angle condition, as it was the case in [3]. We only suppose that  $\beta$  is continuous with the growth bounded from below in the case where the discrete maximum principle is satisfied. In the general case we require in addition  $\beta$  to be

bounded on some interval and Lipschitz-continuous outside this interval. There is no restriction on the maximal time step in the case where F is nondecreasing. If F does not posses this property, we impose an appropriate maximal time step condition. For the sake of simplicity, we only consider the case of a homogeneous Dirichlet boundary condition. Extensions to other types of boundary conditions and to the case where the equation (1.1) involves a nonlinear convection term are possible, using the techniques from [23] and [25]. Finally, this paper is a detailed description of the results previously announced in [28].

The rest of the paper is organized as follows. In Section 2 we state the assumptions on the data and present a weak formulation of the continuous problem. In Section 3 we define the approximation spaces and introduce the combined finite volume–nonconforming/mixed-hybrid finite element scheme. In Section 4 we present some properties of this scheme and prove that it possesses a unique solution, which satisfies the discrete maximum principle under the hypotheses stated above. In Section 5 we derive a priori estimates and estimates on differences of time and space translates for the approximate solutions. Finally, in Section 6, using the Kolmogorov relative compactness theorem, we prove the convergence of a subsequence of the sequence of approximate solutions to a weak solution of the continuous problem. We finally present the results of numerical experiments in Section 7 and give some technical lemmas in Appendix 8.

## 2 The nonlinear degenerate parabolic problem

Let  $\Omega \subset \mathbb{R}^d$ , d = 2, 3, be a polygonal (we use this term for d = 3 as well instead of polyhedral) domain (open, bounded, and connected set) with boundary  $\partial \Omega$ , let (0,T),  $0 < T < \infty$ , be a time interval, and let us define  $Q_T := \Omega \times (0,T)$ . We consider the equation (1.1) in  $Q_T$  together with the homogeneous Dirichlet boundary condition

$$c = 0 \quad \text{on } \partial \Omega \times (0, T)$$
 (2.1)

and the initial condition

$$c(\cdot,0) = c_0 \quad \text{in } \Omega \,. \tag{2.2}$$

Suppose that *S* is a domain of  $\mathbb{R}^d$ . We use the standard notation  $L^p(S)$  and  $\mathbf{L}^p(S) = [L^p(S)]^d$  for the Lebesgue spaces on *S*,  $(\cdot, \cdot)_{0,S}$  stands for the  $L^2(S)$  or  $\mathbf{L}^2(S)$  inner product, and  $\|\cdot\|_{0,S}$  for the associated norm. We use dx as the integration symbol for the Lebesgue measure on *S*,  $d\gamma(\mathbf{x})$  for the Lebesgue measure on a hyperplane of *S*, and *dt* for the Lebesgue measure on (0, T). We denote by |S| the *d*-dimensional Lebesgue measure of *S*, by  $|\sigma|$  the (d-1)-dimensional Lebesgue measure of *S*, by  $|\sigma|$  the distances between all pairs of points of *S*. Next,  $H^1(S)$  and  $H_0^1(S)$  are the Sobolev spaces of functions with square-integrable weak derivatives and  $\mathbf{H}(\operatorname{div}, S) = \{\mathbf{v} \in \mathbf{L}^2(S); \nabla \cdot \mathbf{v} \in L^2(S)\}$ . In the subsequent text we will denote by  $C_A$ ,  $c_A$  a constant basically dependent on a quantity *A* but always independent of the discretization parameters *h* and  $\Delta t$  whose definition we shall give later. We make the following assumption on the data:

Assumption (A) (Data)

(A1)  $\beta \in C(\mathbb{R}), \beta(0) = 0$ , is a strictly increasing function such that

$$|\boldsymbol{\beta}(a) - \boldsymbol{\beta}(b)| \ge c_{\boldsymbol{\beta}}|a - b|, \quad c_{\boldsymbol{\beta}} > 0$$

for all  $a, b \in \mathbb{R}$ 

or

- (A2) in addition to (A1), there exists  $P \in \mathbb{R}$ , P > 0, such that  $|\beta(s)| \leq C_{\beta}$  in [-P,P],  $C_{\beta} > 0$ , and  $\beta$  is Lipschitz-continuous with a constant  $L_{\beta}$  on  $(-\infty, -P]$  and  $[P, +\infty)$ ;
- (A3)  $\mathbf{S}_{ij} \in L^{\infty}(Q_T)$ ,  $|\mathbf{S}_{ij}| \leq C_{\mathbf{S}}/d$  a.e. in  $Q_T$ ,  $1 \leq i, j \leq d, C_{\mathbf{S}} > 0$ ,  $\mathbf{S}$  is a symmetric and uniformly positive definite tensor for almost all  $t \in (0,T)$  with a constant  $c_{\mathbf{S}} > 0$ , *i.e.*

$$\mathbf{S}(\mathbf{x},t)\boldsymbol{\eta}\cdot\boldsymbol{\eta} \geq c_{\mathbf{S}}\boldsymbol{\eta}\cdot\boldsymbol{\eta} \qquad \forall \boldsymbol{\eta}\in\mathbb{R}^{d}, for \ a.e. \ (\mathbf{x},t)\in Q_{T}$$

- (A4)  $\mathbf{v} \in L^2(0,T; \mathbf{H}(\operatorname{div}, \Omega)) \cap \mathbf{L}^{\infty}(Q_T)$  satisfies  $\nabla \cdot \mathbf{v} = r \ge 0$  and  $|\mathbf{v}| \le C_{\mathbf{v}}, C_{\mathbf{v}} > 0$ , *a.e.* in  $Q_T$ ;
- (A5) F(0) = 0, F is a nondecreasing, Lipschitz-continuous function with a constant  $L_F$

- (A6) F(0) = 0, F is a Lipschitz-continuous function with a constant  $L_F$  and there holds  $sF(s) \ge 0$  for s < 0 and s > M, M > 0;
- (A7)  $q \in L^2(Q_T)$ , where  $q = r\overline{c}$  with  $\overline{c} \in L^{\infty}(Q_T)$ ,  $0 \leq \overline{c} \leq M$  a.e. in  $Q_T$ ; (A8)  $c_0 \in L^{\infty}(\Omega)$ ,  $0 \leq c_0 \leq M$  a.e. in  $\Omega$ .

Remark 2.1 (Hypotheses on  $\beta$ ) In contaminant transport problems one typically has  $\beta(c) = c + c^{\alpha}$ ,  $\alpha \in (0, 1)$ . Assumption (A1) generalizes this type of functions; we in particular do not limit the number of points where  $\beta'$  explodes. As we shall see, we will be able to prove the convergence of the combined scheme with this assumption only for the case where the discrete maximum principle (cf. Theorem 4.5 below) holds. In the general case we add Assumption (A2), which is however still satisfied by all realistic functions  $\beta$ . Also, it is necessary that the function  $\beta$  was defined for negative values since our scheme can take them in this latter case.

We now give the definition of a weak solution of (1.1)–(2.2), following essentially Knabner and Otto [36].

**Definition 2.1 (Weak solution)** We say that a function c is a weak solution of the problem (1.1)–(2.2) if

- (i)  $c \in L^2(0,T;H_0^1(\Omega))$ ,
- (*ii*)  $\beta(c) \in L^{\infty}(0,T;L^2(\Omega)),$
- (iii) c satisfies the integral equality

$$-\int_{0}^{T}\int_{\Omega}\beta(c)\varphi_{t}\,\mathrm{d}\mathbf{x}\,\mathrm{d}t - \int_{\Omega}\beta(c_{0})\varphi(\cdot,0)\,\mathrm{d}\mathbf{x} + \int_{0}^{T}\int_{\Omega}\mathbf{S}\nabla c\cdot\nabla\varphi\,\mathrm{d}\mathbf{x}\,\mathrm{d}t - \int_{0}^{T}\int_{\Omega}c\mathbf{v}\cdot\nabla\varphi\,\mathrm{d}\mathbf{x}\,\mathrm{d}t + \int_{0}^{T}\int_{\Omega}F(c)\varphi\,\mathrm{d}\mathbf{x}\,\mathrm{d}t = \int_{0}^{T}\int_{\Omega}q\varphi\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$
for all  $\varphi\in L^{2}(0,T;H_{0}^{1}(\Omega))$  with  $\varphi_{t}\in L^{\infty}(Q_{T}), \varphi(\cdot,T)=0.$ 

*Remark 2.2 (Existence of a weak solution)* The existence of at least one weak solution is proved in Theorem 6.2 below.

*Remark 2.3 (Uniqueness of a weak solution)* For a slightly more restrictive hypothesis on the data than that given in Assumption (A), the uniqueness of a weak solution given by Definition 2.1 is guaranteed in [36]. Namely, no time-dependency of the diffusion–dispersion tensor **S** is still required in [36].

# **3** Combined finite volume–nonconforming/mixed-hybrid finite element scheme

We will describe the space and time discretizations, define the approximation spaces, and introduce the combined finite volume–finite element scheme in this section.

## 3.1 Space and time discretizations

In order to discretize the problem (1.1)–(2.2), we perform a triangulation  $\mathscr{T}_h$  of the domain  $\Omega$ , consisting of closed simplices such that  $\overline{\Omega} = \bigcup_{K \in \mathscr{T}_h} K$  and such that if  $K, L \in \mathscr{T}_h, K \neq L$ , then  $K \cap L$  is either an empty set or a common face, edge, or vertex of K and L. We denote by  $\mathscr{E}_h$  the set of all sides, by  $\mathscr{E}_h^{\text{int}}$  the set of all interior sides, by  $\mathscr{E}_h^{\text{ext}}$  the set of all exterior sides, and by  $\mathscr{E}_K$  the set of all the sides of an element  $K \in \mathscr{T}_h$ . We define  $h := \max_{K \in \mathscr{T}_h} \text{diam}(K)$  and make the following shape regularity assumption on the family of triangulations  $\{\mathscr{T}_h\}_h$ :

#### Assumption (B) (Shape regularity of the space mesh)

*There exists a positive constant*  $\kappa_{\mathcal{T}}$  *such that* 

$$\min_{K \in \mathscr{T}_h} \frac{|K|}{\operatorname{diam}(K)^d} \ge \kappa_{\mathscr{T}} \qquad \forall h > 0$$

Let  $\rho_K$  denote the diameter of the largest ball inscribed in *K*. Then in view of the inequalities  $|K| \ge \text{diam}(K)^{d-1}\rho_K/(d-1)d$ ,  $|K| \le (d+1)\text{diam}(K)^{d-1}\rho_K/(d-1)d$  following from geometrical properties of a triangle (tetrahedron) *K*, Assumption (B) is equivalent to the more common requirement of the existence of a constant  $\theta_{\mathcal{T}} > 0$  such that

$$\max_{K \in \mathcal{T}_h} \frac{\operatorname{diam}(K)}{\rho_K} \le \theta_{\mathcal{T}} \qquad \forall h > 0.$$
(3.1)

Our scheme will next use a dual partition  $\mathcal{D}_h$  of  $\Omega$  such that  $\overline{\Omega} = \bigcup_{D \in \mathcal{D}_h} D$ . There is one dual element *D* associated with each side  $\sigma_D \in \mathcal{E}_h$ . We construct it by connecting the barycentres of every  $K \in \mathcal{T}_h$  that contains  $\sigma_D$  through the vertices of  $\sigma_D$ . For  $\sigma_D \in \mathcal{E}_h^{\text{ext}}$ , the contour of *D* is completed by the side  $\sigma_D$  itself. We refer to Fig. 3.1 for the two-dimensional case. We denote by  $Q_D$  the barycentre of the side  $\sigma_D$ . As for the primal mesh, we set  $\mathcal{F}_h, \mathcal{F}_h^{\text{int}}, \mathcal{F}_h^{\text{ext}}$ , and  $\mathcal{F}_D$  for the dual mesh



**Fig. 3.1** Triangles  $K, L \in \mathscr{T}_h$  and dual volumes  $D, E \in \mathscr{D}_h$  associated with edges  $\sigma_D, \sigma_E \in \mathscr{E}_h$ 

sides. We denote by  $\mathscr{D}_h^{int}$  the set of all interior and by  $\mathscr{D}_h^{ext}$  the set of all boundary dual volumes. We finally denote by  $\mathscr{N}(D)$  the set of all adjacent volumes to the volume D,

$$\mathcal{N}(D) := \left\{ E \in \mathscr{D}_h; \exists \sigma \in \mathscr{F}_h^{\text{int}} \text{ such that } \sigma = \partial D \cap \partial E \right\}$$

and remark that

$$|K \cap D| = \frac{|K|}{d+1} \tag{3.2}$$

for each  $K \in \mathscr{T}_h$  and  $D \in \mathscr{D}_h$  such that  $\sigma_D \in \mathscr{E}_K$ . For  $E \in \mathscr{N}(D)$ , we also set  $d_{D,E} := |Q_E - Q_D|$ ,  $\sigma_{D,E} := \partial D \cap \partial E$ , and  $K_{D,E}$  the element of  $\mathscr{T}_h$  such that  $\sigma_{D,E} \subset K_{D,E}$ .

We suppose the partition of the time interval (0,T) such that  $0 = t_0 < ... < t_n < ... < t_N = T$  and define  $\triangle t_n := t_n - t_{n-1}$  and  $\triangle t := \max_{1 \le n \le N} \triangle t_n$ . In the case where Assumption (A5) is satisfied we do not impose any restriction on the time step. When only Assumption (A6) is satisfied, we suppose in addition:

Assumption (C) (Maximum time step for decreasing F)

The following maximum time step condition is satisfied:

$$\triangle t < \frac{c_{\beta}}{L_F}.$$

We define the following finite-dimensional spaces:

$$\begin{aligned} X_h &:= \left\{ \varphi_h \in L^2(\Omega); \, \varphi_h |_K \text{ is linear } \forall K \in \mathscr{T}_h, \\ \varphi_h \text{ is continuous at the points } Q_D, D \in \mathscr{D}_h^{int} \right\}, \\ X_h^0 &:= \left\{ \varphi_h \in X_h; \, \varphi_h(Q_D) = 0 \quad \forall D \in \mathscr{D}_h^{ext} \right\}. \end{aligned}$$

The basis of  $X_h$  is spanned by the shape functions  $\varphi_D, D \in \mathcal{D}_h$ , such that  $\varphi_D(Q_E) = \delta_{DE}, E \in \mathcal{D}_h, \delta$  being the Kronecker delta. We recall that the approximations in these spaces are nonconforming since  $X_h \not\subset H^1(\Omega)$ . We equip  $X_h$  with the semi-norm

$$\|c_h\|_{X_h}^2 := \sum_{K \in \mathscr{T}_h} \int_K |\nabla c_h|^2 \,\mathrm{d}\mathbf{x}\,,$$

which becomes a norm on  $X_h^0$ . We have the following lemma:

**Lemma 3.1** For all  $c_h = \sum_{D \in \mathscr{D}_h} c_D \varphi_D \in X_h$ , one has

$$\sum_{\sigma_{D,E}\in\mathscr{F}_h^{\text{int}}} \operatorname{diam}(K_{D,E})^{d-2} (c_E - c_D)^2 \le \frac{d+1}{2d\kappa_{\mathscr{T}}} \|c_h\|_{X_h}^2,$$
(3.3)

$$\sum_{\sigma_{D,E}\in\mathscr{F}_{h}^{\text{int}}} \frac{|\sigma_{D,E}|}{d_{D,E}} (c_{E} - c_{D})^{2} \leq \frac{d+1}{2(d-1)\kappa_{\mathscr{T}}} \|c_{h}\|_{X_{h}}^{2}.$$
 (3.4)

Proof Obviously,

$$d_{D,E} \leq \frac{\operatorname{diam}(K_{D,E})}{d}, \quad |\sigma_{D,E}| \leq \frac{\operatorname{diam}(K_{D,E})^{d-1}}{d-1}.$$
(3.5)

Thus

$$\sum_{\sigma_{D,E}\in\mathscr{F}_{h}^{\text{int}}} \operatorname{diam}(K_{D,E})^{d-2} (c_{E}-c_{D})^{2} \leq \sum_{\sigma_{D,E}\in\mathscr{F}_{h}^{\text{int}}} \operatorname{diam}(K_{D,E})^{d-2} \left| \nabla c_{h} \right|_{K_{D,E}} \left|^{2} d_{D,E}^{2} \right|_{\mathcal{F}_{h}^{2}}$$
$$\leq \frac{d+1}{2d} \sum_{K\in\mathscr{F}_{h}} \operatorname{diam}(K)^{d} \left| \nabla c_{h} \right|_{K} \left|^{2} \leq \frac{d+1}{2d\kappa_{\mathscr{F}}} \sum_{K\in\mathscr{F}_{h}} \left| \nabla c_{h} \right|_{K} \left|^{2} \right|_{K} = \frac{d+1}{2d\kappa_{\mathscr{F}}} \|c_{h}\|_{X_{h}}^{2},$$

using the fact that the gradient of  $c_h$  is piecewise constant on  $\mathcal{T}_h$ , (3.5), the fact that each simplex  $K \in \mathcal{T}_h$  contains exactly (d+1)d/2 dual sides, and Assumption (B). This proves (3.3). Similarly,

$$\sum_{\boldsymbol{\sigma}_{D,E}\in\mathscr{F}_{h}^{\text{int}}} \frac{|\boldsymbol{\sigma}_{D,E}|}{d_{D,E}} (c_{E} - c_{D})^{2} \leq \sum_{\boldsymbol{\sigma}_{D,E}\in\mathscr{F}_{h}^{\text{int}}} \left| \nabla c_{h} \right|_{K_{D,E}} \left|^{2} d_{D,E} \left| \boldsymbol{\sigma}_{D,E} \right| \\ \leq \frac{d+1}{2(d-1)\kappa_{\mathscr{F}}} \|c_{h}\|_{X_{h}}^{2}. \quad \Box$$

## 3.2 The combined scheme

We are now ready to present the combined scheme.

**Definition 3.1 (Combined scheme)** The fully implicit combined finite volume– nonconforming/mixed-hybrid finite element scheme for the problem (1.1)–(2.2) reads: find the values  $c_D^n$ ,  $D \in \mathcal{D}_h$ ,  $n \in \{0, 1, ..., N\}$ , such that

$$c_D^0 = \frac{1}{|D|} \int_D c_0(\mathbf{x}) \, \mathrm{d}\mathbf{x} \qquad D \in \mathscr{D}_h^{int} \,, \tag{3.6a}$$

$$c_D^n = 0 \qquad D \in \mathscr{D}_h^{ext}, n \in \{0, 1, \dots, N\},$$

$$(3.6b)$$

$$\frac{\beta(c_D^n) - \beta(c_D^{n-1})}{\triangle t_n} |D| - \sum_{E \in \mathscr{D}_h^{int}} \mathbb{S}_{D,E}^n c_E^n + \sum_{E \in \mathscr{N}(D)} v_{D,E}^n \overline{c_{D,E}^n} + F(c_D^n) |D| = q_D^n |D|$$

$$D \in \mathscr{D}_h^{int}, n \in \{1, 2, \dots, N\}.$$
(3.6c)

In (3.6a)–(3.6c) we have denoted

$$v_{D,E}^{n} := \frac{1}{\triangle t_{n}} \int_{t_{n-1}}^{t_{n}} \int_{\sigma_{D,E}} \mathbf{v}(\mathbf{x},t) \cdot \mathbf{n}_{D,E} \, \mathrm{d}\gamma(\mathbf{x}) \, \mathrm{d}t$$

for  $D \in \mathscr{D}_h^{int}$ ,  $E \in \mathscr{N}(D)$ , and  $n \in \{1, 2, ..., N\}$ , with  $\mathbf{n}_{D,E}$  the unit normal vector of the side  $\sigma_{D,E} \in \mathscr{F}_D$ , outward to D, and

$$q_D^n := \frac{1}{\triangle t_n |D|} \int_{t_{n-1}}^{t_n} \int_D q(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \qquad D \in \mathscr{D}_h, n \in \{1, 2, \dots, N\}$$

We refer to the matrix  $\mathbb{S}^n$  of the elements  $\mathbb{S}_{D,E}^n, D, E \in \mathcal{D}_h^{int}$ , at each discrete time  $t_n, n \in \{1, 2, ..., N\}$ , as to the *diffusion matrix*. This matrix, the stiffness matrix of the nonconforming or mixed-hybrid finite element method, is defined below. Finally, we define  $\overline{c_{D,E}^n}$  for  $D \in \mathcal{D}_h^{int}, E \in \mathcal{N}(D)$ , and  $n \in \{1, 2, ..., N\}$  as follows:

$$\overline{c_{D,E}^{n}} := \begin{cases} c_{D}^{n} + \alpha_{D,E}^{n} (c_{E}^{n} - c_{D}^{n}) & \text{if } v_{D,E}^{n} \ge 0\\ c_{E}^{n} + \alpha_{D,E}^{n} (c_{D}^{n} - c_{E}^{n}) & \text{if } v_{D,E}^{n} < 0 \end{cases}$$
(3.7)

Here  $\alpha_{D,E}^n$  is the coefficient of the amount of upstream weighting which is defined by

$$\alpha_{D,E}^{n} := \frac{\max\left\{\min\left\{\mathbb{S}_{D,E}^{n}, \frac{1}{2}|v_{D,E}^{n}|\right\}, 0\right\}}{|v_{D,E}^{n}|}, \quad v_{D,E}^{n} \neq 0.$$
(3.8)

We set  $\alpha_{D,E}^n := 0$  if  $v_{D,E}^n = 0$ . We remark that  $\overline{c_{D,E}^n} = \widehat{c_{D,E}^n} + \operatorname{sign}(v_{D,E}^n)\alpha_{D,E}^n(c_E^n - c_D^n)$ , where  $\widehat{c_{D,E}^n}$  stands for full upstream weighting.

*Remark 3.1 (Numerical flux)* We can easily see from (3.8) that  $0 \le \alpha_{D,E}^n \le 1/2$ , i.e. the numerical flux defined by (3.7) ranges from the full upstream weighting to the centered scheme. The amount of upstream weighting is set with respect to the local proportion of convection and diffusion.

We now turn to the definition of the diffusion matrix. To this purpose, we first set  $1 - c \ln r$ 

$$\widetilde{\mathbf{S}}^n(\mathbf{x}) := \frac{1}{\triangle t_n} \int_{t_{n-1}}^{t_n} \mathbf{S}(\mathbf{x},t) \, \mathrm{d}t \qquad \mathbf{x} \in \Omega, n \in \{1,2,\ldots,N\}.$$

#### Diffusion matrix from the nonconforming method

The diffusion matrix  $\mathbb{S}^n$  given by the stiffness matrix  $\mathbb{P}^n$  of the nonconforming method writes in the form

$$\mathbb{S}_{D,E}^{n} := \mathbb{P}_{D,E}^{n} = -\sum_{K \in \mathscr{T}_{h}} (\mathbf{S}^{n} \nabla \varphi_{E}, \nabla \varphi_{D})_{0,K} \qquad D, E \in \mathscr{D}_{h}, n \in \{1, 2, \dots, N\},$$
(3.9)

where

$$\mathbf{S}^{n}(\mathbf{x}) = \mathbf{S}^{n}(\mathbf{x}) \qquad n \in \{1, 2, \dots, N\}, \mathbf{x} \in \Omega.$$
(3.10)

In fact, the terms  $\mathbb{S}_{D,E}^n$  for  $D \in \mathcal{D}_h^{ext}$  or  $E \in \mathcal{D}_h^{ext}$  do not occur in the scheme (3.6a)–(3.6c). It will however show convenient to define these values.

## Diffusion matrix from the mixed-hybrid method

Using the analytic form of the stiffness matrix  $\mathbb{M}^n$  of the mixed-hybrid method given in Lemma 8.1 in Appendix 8, we can define the diffusion matrix  $\mathbb{S}^n$  by

$$\mathbb{S}_{D,E}^{n} := \mathbb{M}_{D,E}^{n} = -\sum_{K \in \mathscr{T}_{h}} (\mathbf{S}^{n} \nabla \varphi_{E}, \nabla \varphi_{D})_{0,K} \qquad D, E \in \mathscr{D}_{h}, n \in \{1, 2, \dots, N\},$$
(3.11)

where

$$\mathbf{S}^{n}(\mathbf{y}) = \left(\frac{1}{|K|} \int_{K} [\widetilde{\mathbf{S}}^{n}(\mathbf{x})]^{-1} \, \mathrm{d}\mathbf{x}\right)^{-1} \qquad \mathbf{y} \in K, K \in \mathscr{T}_{h}, n \in \{1, 2, \dots, N\}.$$
(3.12)

*Remark 3.2 (Stiffness matrices of nonconforming and mixed-hybrid methods)* We remark that the stiffness matrix of the mixed-hybrid method (3.11) is the stiffness matrix of the nonconforming method (3.9) with a piecewise constant diffusion tensor, given as the inverse of the elementwise average of the inverse of the original one. In particular for an elementwise constant diffusion tensor, the stiffness matrices coincide, whereas for a general diffusion tensor, (3.9) uses its arithmetic and (3.11) its harmonic average.

Remark 3.3 (Comparison with a pure finite volume scheme) Let us consider  $\mathscr{T}_h$  consisting of equilateral simplices and  $\mathbf{S} = Id$ . Then the segments  $[Q_D, Q_E]$  are orthogonal to the dual sides  $\sigma_{D,E}$  and one has  $\mathbb{P}_{D,E}^n = \mathbb{M}_{D,E}^n = \frac{|\sigma_{D,E}|}{d_{D,E}}$ ,  $E \in \mathscr{N}(D)$ . Thus, in view of Corollary 4.1 below, the pure cell-centered finite volume scheme completely coincides in this case with the combined one. One may regard in this sense the combined scheme as an extension of the pure finite volume scheme to general triangulations and full-matrix diffusion tensors, which does not extend the original 5-point (7-point in space dimension three) stencil.

Remark 3.4 (Comparison of a combined finite volume–finite element scheme with pure finite volume schemes) We recall that for triangular meshes, the discretization of a Laplacian by the piecewise linear conforming finite element method coincides with that by the vertex-centered finite volume method [2, 38], which is also named the box scheme [6], the finite volume element scheme [13], or the control volume finite element scheme [31], see [6, Lemma 3]. Finally, for Delaunay triangulations (the sums of two opposite angles to all edges are less or equal to  $\pi$ ), constructing the control volumes with the aid of orthogonal bisectors, these discretizations are equivalent to that by the cell-centered finite volume method, see [23, Section III.12]. Hence, when  $\mathbf{S} = Id$  and for a Delaunay triangular mesh with the above construction of control volumes, the combined finite volume–finite element scheme [30], the vertex-centered finite volume scheme [2,38], and the cell-centered finite volume scheme [23,25] for the discretization of (1.1) coincide.

In the sequel we shall consider apart the following special case:

## Assumption (D) (Diffusion matrix)

All transmissibilities are non-negative, i.e.

$$\mathbb{S}_{D,E}^{n} \ge 0 \qquad \forall D \in \mathscr{D}_{h}^{int}, E \in \mathscr{N}(D) \qquad \forall n \in \{1, 2, \dots, N\}$$

Since

$$\nabla \varphi_D|_K = \frac{|\sigma_D|}{|K|} \mathbf{n}_{\sigma_D} \qquad K \in \mathscr{T}_h, \, \sigma_D \in \mathscr{E}_K \tag{3.13}$$

with  $\mathbf{n}_{\sigma_D}$  the unit normal vector of the side  $\sigma_D$ , outward to K, one can immediately see that Assumption (D) is satisfied e.g. when the diffusion tensor reduces to a scalar function and when the magnitude of the angles between  $\mathbf{n}_{\sigma_D}$ ,  $\sigma_D \in \mathscr{E}_K$ , for all  $K \in \mathscr{T}_h$  is greater or equal to  $\pi/2$  (all interior angles smaller or equal to  $\pi/2$  in two space dimensions).

#### 4 Existence, uniqueness, and discrete properties

In this section we first present some technical lemmas. We then show the conservativity of the scheme, the coercivity of the bilinear diffusion form corresponding to the diffusion term, and an a priori estimate for an extended scheme, which is needed later in the proof of the existence of the solution of the discrete problem. Finally, we prove the uniqueness of this solution and the discrete maximum principle when Assumption (D) is satisfied.

#### 4.1 Discrete properties of the scheme

**Lemma 4.1** (Nonconforming finite element diffusion matrix) For all  $D \in \mathcal{D}_h$ and  $n \in \{1, 2, ..., N\}$ ,  $\mathbb{S}_{D,D}^n = -\sum_{E \in \mathcal{N}(D)} \mathbb{S}_{D,E}^n$ .

*Proof* We will show the assertion for d = 2; the case d = 3 is similar. We present the proof for the nonconforming method, which in view of Remark 3.2 implies the same result for the mixed-hybrid method. Let us consider a fixed dual volume  $D \in \mathscr{D}_h$ . The edge  $\sigma_D$  associated with *D* is shared by at most two triangles, which we denote by *K* and *L*. The sum over  $K \in \mathscr{T}_h$  in (3.9) for  $\mathbb{S}_{D,D}^n$  reduces just to these triangles, considering the definition of the basis function  $\varphi_D$ . We denote the dual volumes associated with the two other edges of *L* by  $E_1$  and  $E_2$ . Similarly, the sum over  $K \in \mathscr{T}_h$  in (3.9) for  $\mathbb{S}_{D,E_1}^n$  and  $\mathbb{S}_{D,E_2}^n$  reduces to *L*. Thus it is sufficient to prove that

$$-(\mathbf{S}^n \nabla \varphi_D, \nabla \varphi_D)_{0,L} = (\mathbf{S}^n \nabla \varphi_{E_1}, \nabla \varphi_D)_{0,L} + (\mathbf{S}^n \nabla \varphi_{E_2}, \nabla \varphi_D)_{0,L},$$

since the eventual contribution of the element K is similar. However, this is immediate, since

$$-\varphi_D|_L = (\varphi_{E_1} + \varphi_{E_2})|_L - 1$$
.  $\Box$ 

**Corollary 4.1 (Equivalent form of the diffusion term)** Let  $D \in \mathcal{D}_h$ . Using the fact that  $\mathbb{S}_{D,E}^n \neq 0$  only if  $E \in \mathcal{N}(D)$  or if E = D and Lemma 4.1, one has

$$\sum_{E \in \mathscr{D}_h} \mathbb{S}_{D,E}^n c_E^n = \sum_{E \in \mathscr{N}(D)} \mathbb{S}_{D,E}^n c_E^n + \mathbb{S}_{D,D}^n c_D^n = \sum_{E \in \mathscr{N}(D)} \mathbb{S}_{D,E}^n (c_E^n - c_D^n)$$

**Theorem 4.1 (Conservativity of the scheme)** The scheme (3.6a)–(3.6c) is conservative with respect to the dual mesh  $\mathcal{D}_h$ .

*Proof* The proof given here uses the "finite volume interpretation", cf. [23]. "Finite element interpretations" exist as well, cf. [32].

First, the equation (3.6c) defining the scheme and Corollary 4.1 imply that the combined finite volume–finite element scheme is conservative on each time level and on each cell of the dual mesh as the pure finite volume is—the sum of the fluxes over the sides of each dual cell equals the time-accumulation, sources, and reaction term in this cell.

We next address the continuity of the fluxes across each dual side. To this purpose, we first notice that on each time level, the approximate solution  $c_h^n = \sum_{D \in \mathscr{D}_h} c_D^n \varphi_D \in X_h^0$  is continuous over the dual mesh sides together with its gradient. Alternatively, for the discrete diffusive flux, we can argue as follows. Let us take two fixed neighboring dual volumes *E* and *D*,  $D \in \mathscr{D}_h^{int}$ . Using Corollary 4.1 and (3.6b), the discrete diffusive flux from *D* to *E* can be expressed as  $-\mathbb{S}_{D,E}^n(c_E^n - c_D^n)$ . The discrete diffusive flux from *E* to *D* is  $-\mathbb{S}_{E,D}^n(c_D^n - c_E^n)$ , i.e. we have their equality up to the sign, considering that  $\mathbb{S}_{D,E}^n = \mathbb{S}_{E,D}^n$  for all  $n \in \{1, 2, ..., N\}$ , which follows from (3.9) or (3.11) using the symmetry of the tensor **S**. Hence the discrete diffusive flux is conservative.

For the discrete convective flux from *D* to *E*, we have  $v_{D,E}^n[c_D^n + \alpha_{D,E}^n(c_E^n - c_D^n)]$ , supposing  $v_{D,E}^n \ge 0$ . For this flux from *E* to *D*, we have  $v_{E,D}^n[c_D^n + \alpha_{E,D}^n(c_E^n - c_D^n)]$ , i.e. again the equality up to the sign, considering that  $v_{D,E}^n = -v_{E,D}^n$  and that  $\alpha_{D,E}^n = \alpha_{E,D}^n$ , which follows from  $\mathbb{S}_{D,E}^n = \mathbb{S}_{E,D}^n$ . For  $v_{D,E}^n < 0$ , the proof is similar. Hence the discrete convective flux is conservative as well.  $\Box$ 

**Lemma 4.2 (Equivalent form of the upwind part of the convection term**) *For* all  $D \in \mathcal{D}_h^{int}$  and  $n \in \{1, 2, ..., N\}$ ,

$$\sum_{E\in\mathscr{N}(D)} v_{D,E}^n \ \widehat{c_{D,E}^n} = \sum_{E\in\mathscr{N}(D)} (v_{D,E}^n)^- (c_E^n - c_D^n) + r_D^n c_D^n |D| \,,$$

where  $(v_{D,E}^{n})^{-} := \min\{v_{D,E}^{n}, 0\}$  and

$$r_D^n := \frac{1}{\triangle t_n |D|} \int_{t_{n-1}}^{t_n} \int_D r(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \qquad \forall D \in \mathscr{D}_h, \, \forall n \in \{1, 2, \dots, N\}.$$

The assertion of this lemma is a simple consequence of Assumption (A4). The proof can be found in [41].

**Lemma 4.3** (Coercivity of the diffusion form) For all  $c_h = \sum_{D \in \mathscr{D}_h} c_D \varphi_D \in X_h$  and  $n \in \{1, 2, ..., N\}$ ,

$$-\sum_{D\in\mathscr{D}_h} c_D \sum_{E\in\mathscr{D}_h} \mathbb{S}_{D,E}^n c_E \ge c_{\mathbf{S}} \|c_h\|_{X_h}^2$$

Proof We have

$$-\sum_{D\in\mathscr{D}_h} c_D \sum_{E\in\mathscr{D}_h} \mathbb{S}_{D,E}^n c_E = \sum_{K\in\mathscr{T}_h} (\mathbf{S}^n \nabla c_h, \nabla c_h)_{0,K} \ge c_{\mathbf{S}} \|c_h\|_{X_h}^2,$$

using (3.9) or (3.11) and Assumption (A3) and the subsequent uniform positive definiteness of the diffusion tensors (3.10) and (3.12).  $\Box$ 

**Lemma 4.4 (Boundedness of the diffusion form)** For all  $c_h = \sum_{D \in \mathscr{D}_h} c_D \varphi_D \in X_h$ and  $n \in \{1, 2, ..., N\}$ ,

$$-\sum_{D\in\mathscr{D}_h} c_D \sum_{E\in\mathscr{D}_h} \mathbb{S}_{D,E}^n c_E \bigg| \le C_{\mathbf{S}} \|c_h\|_{X_h}^2.$$

$$(4.1)$$

*Moreover, for all*  $D \in \mathcal{D}_h$ ,  $E \in \mathcal{N}(D)$ , and  $n \in \{1, 2, ..., N\}$ ,

$$|\mathbb{S}_{D,E}^{n}| \leq \frac{C_{\mathbf{S}}}{\kappa_{\mathscr{T}}} \frac{\operatorname{diam}(K_{D,E})^{d-2}}{(d-1)^{2}}.$$
(4.2)

The assertion of this lemma is a simple consequence of Assumption (A3) and of (3.13). The proof can be found in [41].

**Lemma 4.5 (Estimate on the convection term)** For all values  $c_D$ ,  $D \in \mathcal{D}_h$ , such that  $c_D = 0$  for all  $D \in \mathcal{D}_h^{ext}$  and  $n \in \{1, 2, ..., N\}$ ,

$$\sum_{D\in \mathscr{D}_h^{int}} c_D \sum_{E\in \mathscr{N}(D)} v_{D,E}^n \ \overline{c_{D,E}} \geq 0$$

Proof We can write

$$\begin{split} &\sum_{D\in\mathscr{T}_{h}^{int}}c_{D}\sum_{E\in\mathscr{N}(D)}v_{D,E}^{n}\overline{c_{D,E}}\\ &=\sum_{\sigma_{D,E}\in\mathscr{T}_{h}^{int},v_{D,E}^{n}\geq0}v_{D,E}^{n}\left(c_{D}(c_{D}-c_{E})-\alpha_{D,E}^{n}(c_{E}-c_{D})^{2}\right)\\ &=\frac{1}{2}\sum_{\sigma_{D,E}\in\mathscr{T}_{h}^{int},v_{D,E}^{n}\geq0}v_{D,E}^{n}(c_{D}^{2}-c_{E}^{2})+\sum_{\sigma_{D,E}\in\mathscr{T}_{h}^{int}}|v_{D,E}^{n}|(c_{E}-c_{D})^{2}\left(\frac{1}{2}-\alpha_{D,E}^{n}\right)\\ &\geq\frac{1}{2}\sum_{D\in\mathscr{T}_{h}^{int}}c_{D}^{2}\sum_{E\in\mathscr{N}(D)}v_{D,E}^{n}=\frac{1}{2}\sum_{D\in\mathscr{T}_{h}^{int}}c_{D}^{2}r_{D}^{n}|D|\geq0, \end{split}$$

where we have used the fact that  $c_D = 0$  for all  $D \in \mathscr{D}_h^{ext}$ , the relation  $2(a-b)a = (a-b)^2 + a^2 - b^2$ , and rewritten the summation over interior dual sides with fixed denotation of the dual volumes sharing given side  $\sigma_{D,E}$  such that  $v_{D,E}^n \ge 0$ . In the last two estimates we have used, respectively, the fact that  $0 \le \alpha_{D,E}^n \le 1/2$ , which follows from (3.8), and Assumption (A4).  $\Box$ 

**Theorem 4.2 (A priori estimate for an extended scheme)** *Let us define an extended scheme by* 

$$c_D^0 = \frac{1}{|D|} \int_D c_0(\mathbf{x}) \, \mathrm{d}\mathbf{x} \qquad D \in \mathscr{D}_h^{int} \,, \tag{4.3a}$$

$$c_D^n = 0$$
  $D \in \mathcal{D}_h^{ext}, n \in \{0, 1, \dots, N\},$  (4.3b)

$$u \frac{\beta(c_D^n) - \beta(c_D^{n-1})}{\Delta t_n} |D| - \sum_{E \in \mathscr{D}_h^{int}} \mathbb{S}_{D,E}^n c_E^n + u \sum_{E \in \mathscr{N}(D)} v_{D,E}^n \overline{c_{D,E}^n} + u F(c_D^n) |D|$$
$$= u q_D^n |D| \qquad D \in \mathscr{D}_h^{int}, n \in \{1, 2, \dots, N\}$$
(4.3c)

with  $u \in [0,1]$ . Then

$$\sum_{D \in \mathscr{D}_h} (c_D^n)^2 |D| \le C_{\text{es}} \qquad \forall n \in \{1, 2, \dots, N\}$$

with

$$C_{\rm es} := \frac{8}{c_\beta} M\beta(M) |\Omega| + \frac{16T}{c_\beta^2} ||q||_{0,Q_T}^2 + \frac{8}{c_\beta} L_F M^2 T |\Omega|.$$

*Proof* We multiply (4.3c) by  $\triangle t_n c_D^n$ , sum over all  $D \in \mathcal{D}_h^{int}$  and  $n \in \{1, 2, \dots, k\}$ , and use the fact that  $u \ge 0$  and Lemmas 4.3 and 4.5. Further, for  $c_D^n < 0$  or  $c_D^n > M$ ,  $F(c_D^n)c_D^n \ge 0$  follows from Assumption (A5) or (A6). When  $0 \le c_D^n \le M$ ,  $-F(c_D^n)c_D^n \le |F(c_D^n)||c_D^n| \le L_F M^2$ , which altogether yields

$$u\sum_{n=1}^{k}\sum_{D\in\mathscr{D}_{h}^{int}}[\beta(c_{D}^{n})-\beta(c_{D}^{n-1})]c_{D}^{n}|D|+c_{\mathbf{S}}\sum_{n=1}^{k}\bigtriangleup t_{n}\|c_{h}^{n}\|_{X_{h}}^{2}$$

$$\leq u\sum_{n=1}^{k}\bigtriangleup t_{n}\sum_{D\in\mathscr{D}_{h}^{int}}c_{D}^{n}q_{D}^{n}|D|+uL_{F}M^{2}\sum_{n=1}^{k}\sum_{D\in\mathscr{D}_{h}^{int}}\bigtriangleup t_{n}|D|$$

$$(4.4)$$

with  $c_h^n = \sum_{D \in \mathscr{D}_h} c_D^n \varphi_D$ . Let us now introduce a function *B*,

$$B(s) := eta(s)s - \int_0^s eta( au) \,\mathrm{d} au \qquad s \in \mathbb{R}$$

One then can derive

$$B(c_D^n) - B(c_D^{n-1}) = [\beta(c_D^n) - \beta(c_D^{n-1})]c_D^n - \int_{c_D^{n-1}}^{c_D^n} [\beta(\tau) - \beta(c_D^{n-1})] d\tau.$$

Using that  $\beta$  is nondecreasing, one can easily show that

$$\int_{c_D^{n-1}}^{c_D^n} [\beta(\tau) - \beta(c_D^{n-1})] \,\mathrm{d}\tau \ge 0$$

In view of the two last expressions, one has

$$\sum_{n=1}^{k} \sum_{D \in \mathscr{D}_{h}^{int}} [B(c_{D}^{n}) - B(c_{D}^{n-1})] |D| \leq \sum_{n=1}^{k} \sum_{D \in \mathscr{D}_{h}^{int}} [\beta(c_{D}^{n}) - \beta(c_{D}^{n-1})] c_{D}^{n} |D|,$$

which yields

$$\sum_{D\in\mathscr{D}_h^{int}} B(c_D^k)|D| - \sum_{D\in\mathscr{D}_h^{int}} B(c_D^0)|D| \le \sum_{n=1}^k \sum_{D\in\mathscr{D}_h^{int}} [\beta(c_D^n) - \beta(c_D^{n-1})]c_D^n|D|.$$

Using the growth condition on  $\beta$  from Assumption (A1), one can derive  $B(s) \ge s^2 c_\beta/2$  for all  $s \in \mathbb{R}$ , see Lemma 8.2 in Appendix 8. Thus, using in addition Assumption (A8)

$$\frac{c_{\beta}}{2}\sum_{D\in\mathscr{D}_{h}^{int}}(c_{D}^{k})^{2}|D|-M\beta(M)|\Omega|\leq \sum_{n=1}^{k}\sum_{D\in\mathscr{D}_{h}^{int}}[\beta(c_{D}^{n})-\beta(c_{D}^{n-1})]c_{D}^{n}|D|.$$

We notice that

$$\sum_{n=1}^{N} \sum_{D \in \mathscr{D}_h} \triangle t_n |D| (q_D^n)^2 \le ||q||_{0,Q_T}^2$$
(4.5)

by the Cauchy–Schwarz inequality. Hence extending the summation over all  $n \in \{1, 2, ..., N\}$  and  $D \in \mathcal{D}_h$  in the first term of the right-hand side of (4.4) and using the Cauchy–Schwarz and Young inequality, we have

$$\begin{split} \sum_{n=1}^{k} \triangle t_n \sum_{D \in \mathscr{D}_h^{int}} c_D^n q_D^n |D| &\leq \left( \sum_{n=1}^{N} \triangle t_n \sum_{D \in \mathscr{D}_h} (c_D^n)^2 |D| \right)^{\frac{1}{2}} \|q\|_{0,\mathcal{Q}_T} \\ &\leq \frac{\varepsilon}{2} \sum_{n=1}^{N} \triangle t_n \sum_{D \in \mathscr{D}_h} (c_D^n)^2 |D| + \frac{1}{2\varepsilon} \|q\|_{0,\mathcal{Q}_T}^2. \end{split}$$

Hence, substituting these estimates into (4.4), we obtain

$$u\frac{c_{\beta}}{2} \max_{n \in \{1,2,\dots,N\}} \sum_{D \in \mathscr{D}_{h}} (c_{D}^{n})^{2} |D| + c_{\mathbf{S}} \sum_{n=1}^{N} \triangle t_{n} \|c_{h}^{n}\|_{X_{h}}^{2} \leq 2uM\beta(M) |\Omega| \quad (4.6)$$
$$+ u\varepsilon T \max_{n \in \{1,2,\dots,N\}} \sum_{D \in \mathscr{D}_{h}} (c_{D}^{n})^{2} |D| + u\frac{1}{\varepsilon} \|q\|_{0,Q_{T}}^{2} + 2uL_{F}M^{2}T |\Omega|,$$

considering also (4.3b) and the fact that *k* was arbitrarily chosen. We now put  $\varepsilon = c_{\beta}/(4T)$ . When  $u \neq 0$ , this already yields the assertion of the lemma. When u = 0, it follows from (4.6) that  $c_D^n = 0$  for all  $D \in \mathcal{D}_h$  and all  $n \in \{1, 2, ..., N\}$ , since in view of (4.3b),  $\|\cdot\|_{X_h}$  is a norm on  $X_h$ . Thus the assertion of the lemma is trivially satisfied in this case.  $\Box$ 

4.2 Existence, uniqueness, and the discrete maximum principle

**Theorem 4.3 (Existence of the solution of the discrete problem)** *The problem* (3.6a)–(3.6c) has at least one solution.

The proof follows the ideas of the proof given in [27]. It makes use of the a priori estimate for the extended scheme given by Theorem 4.2 and of the (Brouwer) topological degree argument. It can be found in [41].

**Theorem 4.4** (Uniqueness of the solution of the discrete problem) *The solution of the problem* (3.6a)–(3.6c) *is unique.* 

*Proof* We will prove the assertion by contradiction. Let us thus suppose that there exists  $n \in \{1, 2, ..., N\}$  such that  $c_D^{n-1} = \tilde{c}_D^{n-1}$  for all  $D \in \mathscr{D}_h^{int}$  but  $c_D^n \neq \tilde{c}_D^n$  for some  $D \in \mathscr{D}_h^{int}$ . After subtracting the equation (3.6c) for  $c_D^n$  and  $\tilde{c}_D^n$  and denoting  $s_D^n := c_D^n - \tilde{c}_D^n$ , we have

$$\frac{\beta(c_D^n) - \beta(\tilde{c}_D^n)}{\triangle t_n} |D| - \sum_{E \in \mathscr{D}_h^{int}} \mathbb{S}_{D,E}^n s_E^n + \sum_{E \in \mathscr{N}(D)} v_{D,E}^n \overline{s_{D,E}^n} + F(c_D^n) |D| - F(\tilde{c}_D^n) |D| = 0 \qquad D \in \mathscr{D}_h^{int},$$

where  $\overline{s_{D,E}^n}$  is given by (3.7) while changing *c* by *s*. We now multiply the above equality by  $s_D^n$  and sum the result over  $D \in \mathcal{D}_h^{int}$ . This yields, using Lemmas 4.3 and 4.5,

$$\sum_{D \in \mathscr{D}_h^{int}} [\beta(c_D^n) - \beta(\tilde{c}_D^n)](c_D^n - \tilde{c}_D^n) \frac{|D|}{\Delta t_n} + \sum_{D \in \mathscr{D}_h^{int}} [F(c_D^n) - F(\tilde{c}_D^n)](c_D^n - \tilde{c}_D^n) |D| \le 0.$$

When Assumption (A5) is satisfied, this is already a contradiction, since from Assumption (A1),  $\beta$  is strictly increasing and *F* is nondecreasing in this case.

When only Assumption (A6) is satisfied, we have  $|-[F(c_D^n) - F(\tilde{c}_D^n)](c_D^n - \tilde{c}_D^n)| \le L_F(c_D^n - \tilde{c}_D^n)^2$ . In view of Assumption (A1),  $[\beta(c_D^n) - \beta(\tilde{c}_D^n)](c_D^n - \tilde{c}_D^n) \ge c_\beta(c_D^n - \tilde{c}_D^n)^2$ . Since

$$\sum_{D\in\mathscr{D}_h^{int}} (c_D^n - \tilde{c}_D^n)^2 |D| \neq 0,$$

 $c_{\beta}/L_F \leq \Delta t_n$ , which is a contradiction with Assumption (C) supposed in this case.  $\Box$ 

**Theorem 4.5 (Discrete maximum principle)** Under Assumption (D), the solution of the problem (3.6a)–(3.6c) satisfies

$$0 \le c_D^n \le M$$

for all  $D \in \mathcal{D}_h$ ,  $n \in \{1, 2, \dots, N\}$ .

*Proof* Setting  $\mathbb{T}_{D,E}^n := \mathbb{S}_{D,E}^n - |v_{D,E}^n| \alpha_{D,E}^n, D \in \mathcal{D}_h^{int}, E \in \mathcal{N}(D)$ , and using Corollary 4.1 and Lemma 4.2, we can rewrite (3.6c) as

$$\frac{\beta(c_D^n) - \beta(c_D^{n-1})}{\Delta t_n} |D| - \sum_{E \in \mathcal{N}(D)} \mathbb{T}_{D,E}^n(c_E^n - c_D^n) + \sum_{E \in \mathcal{N}(D)} (v_{D,E}^n)^- (c_E^n - c_D^n) + r_D^n c_D^n |D| + F(c_D^n) |D| = q_D^n |D| \qquad D \in \mathcal{D}_h^{int}, n \in \{1, 2, \dots, N\}.$$
(4.7)

In view of Assumption (D) and of (3.8), one has  $\mathbb{T}_{D,E}^n \ge 0$  for all  $D \in \mathcal{D}_h^{int}$ ,  $E \in \mathcal{N}(D)$ , and  $n \in \{1, 2, ..., N\}$ . We now make use of an induction argument. We remark that  $0 \le c_D^n \le M$  is satisfied for n = 0 by Assumption (A8) and (3.6a) and (3.6b). Let us suppose that  $0 \le c_D^{n-1} \le M$  for all  $D \in \mathcal{D}_h^{int}$  and for a fixed  $(n-1) \in \{0, 1, ..., N-1\}$ . Since  $|\mathcal{D}_h|$  is finite, there exist  $D_0, D_1 \in \mathcal{D}_h$  such that  $c_{D_0}^n \le c_D^n \le c_{D_1}^n$  for all  $D \in \mathcal{D}_h$ . Using a contradiction argument we prove below

that  $c_{D_0}^n \ge 0$  and  $c_{D_1}^n \le M$ . Suppose that  $c_{D_0}^n < 0$ . We remark that  $D_0 \in \mathscr{D}_h^{int}$  because of (3.6b). Then, since  $\mathbb{T}_{D_0,E}^n \ge 0$  and  $-(v_{D_0,E}^n)^- \ge 0$ , we have

$$\sum_{E \in \mathscr{N}(D_0)} \mathbb{T}_{D_0,E}^n(c_E^n - c_{D_0}^n) + \sum_{E \in \mathscr{N}(D_0)} - (v_{D_0,E}^n)^-(c_E^n - c_{D_0}^n) \ge 0.$$

This yields, using (4.7),

$$\frac{\beta(c_{D_0}^n) - \beta(c_{D_0}^{n-1})}{\Delta t_n} |D_0| + r_{D_0}^n c_{D_0}^n |D_0| + F(c_{D_0}^n) |D_0| - q_{D_0}^n |D_0| \ge 0.$$

Now  $c_{D_0}^n < 0$  implies  $r_{D_0}^n c_{D_0}^n \le 0$  and  $F(c_{D_0}^n) \le 0$  using, respectively, Assumption (A4) and (A5) or (A6). Also  $-q_{D_0}^n \le 0$ , using Assumption (A7). Hence  $\beta(c_{D_0}^n) \ge \beta(c_{D_0}^{n-1})$ , which is a contradiction, since  $\beta$  is strictly increasing from Assumption (A1).

Let us now suppose  $c_{D_1}^n > M$ . Again  $D_1 \in \mathscr{D}_h^{int}$ , because of (3.6b). Similarly as in the previous case, one comes to

$$\frac{\beta(c_{D_1}^n) - \beta(c_{D_1}^{n-1})}{\triangle t_n} |D_1| + r_{D_1}^n c_{D_1}^n |D_1| + F(c_{D_1}^n) |D_1| - q_{D_1}^n |D_1| \le 0.$$

We can estimate

$$-q_{D_1}^n |D_1| \ge -Mr_{D_1}^n |D_1| \ge -c_{D_1}^n r_{D_1}^n |D_1|$$

using, respectively, Assumption (A7) and (A4). It follows from (A5) or (A6) that  $F(c_{D_1}^n) \ge 0$ . This implies  $\beta(c_{D_1}^n) \le \beta(c_{D_1}^{n-1})$ , which is again a contradiction, using Assumption (A1).  $\Box$ 

#### 5 A priori estimates

In this section we give a priori estimates and estimates on differences of time and space translates of the approximate solutions that we shall define.

#### 5.1 Discrete energy-type estimates

We now give energy-type estimates for the approximate solution values  $c_D^n$ ,  $D \in \mathcal{D}_h$ ,  $n \in \{0, 1, ..., N\}$ .

**Theorem 5.1** (A priori estimates) *The solution of the combined scheme* (3.6a)–(3.6c) *satisfies* 

$$c_{\beta} \max_{n \in \{1,2,\dots,N\}} \sum_{D \in \mathscr{D}_h} (c_D^n)^2 |D| \le C_{\text{ae}}, \qquad (5.1)$$

$$\max_{n \in \{1,2,\dots,N\}} \sum_{D \in \mathscr{D}_h} [\beta(c_D^n)]^2 |D| \le C_{\mathrm{ae}\beta} , \qquad (5.2)$$

$$c_{\mathbf{S}}\sum_{n=1}^{N} \triangle t_n \|c_h^n\|_{X_h}^2 \le C_{\mathrm{ae}}$$

$$(5.3)$$

with  $c_h^n = \sum_{D \in \mathscr{D}_h} c_D^n \varphi_D$ ,  $C_{ae} := 8M\beta(M)|\Omega| + \frac{16T}{c_\beta} ||q||_{0,Q_T}^2 + 8L_F M^2 T |\Omega|$ ,  $C_{ae\beta} := [\beta(M)]^2 |\Omega|$ 

when Assumption (D) is satisfied and only Assumption (A1) holds and

$$C_{\mathrm{ae}\beta} := (2C_{\beta}^2 + 4L_{\beta}^2 P^2)|\Omega| + \frac{4L_{\beta}^2}{c_{\beta}}C_{\mathrm{ae}}$$

when Assumption (D) is not satisfied but Assumption (A2) holds.

*Proof* Estimates (5.1) and (5.3) follow immediately from (4.6) for  $\varepsilon = c_{\beta}/(4T)$ , since for u = 1 the extended scheme (4.3a)–(4.3c) completely coincides with the scheme (3.6a)–(3.6c). To see the boundedness of the term on the left-hand side of (5.2) under Assumption (D) is immediate, using the discrete maximum principle stated by Theorem 4.5. In this case Assumption (A1) suffices. In the general case one has to use Assumption (A2) to show  $[\beta(s)]^2 \leq 2C_{\beta}^2 + 4L_{\beta}^2P^2 + 4L_{\beta}^2s^2$ , see Lemma 8.3 in Appendix 8. Hence, for all  $n \in \{1, 2, ..., N\}$ ,

$$\sum_{D\in\mathscr{D}_h} [\beta(c_D^n)]^2 |D| \le (2C_\beta^2 + 4L_\beta^2 P^2) |\Omega| + 4L_\beta^2 \sum_{D\in\mathscr{D}_h} (c_D^n)^2 |D|. \quad \Box$$

Using the values  $c_D^n$ ,  $D \in \mathcal{D}_h$ ,  $n \in \{0, 1, ..., N\}$ , we now define two approximate solutions.

**Definition 5.1 (Approximate solutions)** Let the values  $c_D^n$  with  $D \in \mathcal{D}_h$ ,  $n \in \{0, 1, ..., N\}$ , be the solutions to (3.6a)–(3.6c). As the approximate solutions of the problem (1.1)–(2.2) by means of the combined finite volume–nonconforming/mi-xed-hybrid finite element scheme, we understand:

(i) The function  $c_{h, \triangle t}$  defined by

$$c_{h,\Delta t}(\mathbf{x},0) = c_h^0(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega,$$
  

$$c_{h,\Delta t}(\mathbf{x},t) = c_h^n(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega, t \in (t_{n-1},t_n] \qquad n \in \{1,\dots,N\}, \quad (5.4)$$

where  $c_h^n = \sum_{D \in \mathscr{D}_h} c_D^n \varphi_D;$ 

(ii) The function  $\tilde{c}_{h, \Delta t}$  defined by

$$\begin{aligned} \tilde{c}_{h,\triangle t}(\mathbf{x},0) &= c_D^0 \text{ for } \mathbf{x} \in D^\circ, D \in \mathscr{D}_h, \\ \tilde{c}_{h,\triangle t}(\mathbf{x},t) &= c_D^n \text{ for } \mathbf{x} \in D^\circ, D \in \mathscr{D}_h, t \in (t_{n-1},t_n] \qquad n \in \{1,\ldots,N\}. \end{aligned}$$

The function  $c_{h,\triangle t}$  is piecewise linear and continuous in the barycentres of the interior sides in space and piecewise constant in time; we will call it a *nonconforming finite element solution*. The function  $\tilde{c}_{h,\triangle t}$  is given by the values of  $c_{h,\triangle t}$  in side barycentres and is piecewise constant on the dual volumes in space and piecewise constant in time; we will call it a *finite volume solution*. The following important relation between  $c_{h,\triangle t}$  and  $\tilde{c}_{h,\triangle t}$  is a simple consequence of the a priori estimate (5.3) (for the proof, see [41]):

**Lemma 5.1** (Relation between  $c_{h, \Delta t}$  and  $\tilde{c}_{h, \Delta t}$ ) There holds

$$||c_{h, \triangle t} - \tilde{c}_{h, \triangle t}||_{0, Q_T} \longrightarrow 0 \text{ as } h \rightarrow 0.$$

*Remark 5.1 (Interpretation of the values*  $c_D^n$ ) We remark that the approximate solutions  $c_{h, \triangle t}$  and  $\tilde{c}_{h, \triangle t}$  are only interpretations of the values  $c_D^n$ ,  $D \in \mathcal{D}_h$ ,  $n \in \{0, 1, \dots, N\}$ . In particular, we may work with  $\tilde{c}_{h, \triangle t}$  as in the finite volume method and then use Lemma 5.1 to extend the convergence results also to  $c_{h, \triangle t}$ .

5.2 Estimates on differences of time and space translates

Estimates on differences of time and space translates have been used in [26,27] to prove the relative compactness property of the sequence of approximate solutions. We give below the time translate estimate for  $\tilde{c}_{h,\Delta t}$  given by (5.5). We extend the techniques from [26,27] to the case of transmissibilities issued from the nonconforming/mixed-hybrid finite element method, which may in particular be negative (this implies that the discrete maximum principle is not satisfied), and to a nonconstant time step.

**Lemma 5.2** (Time translate estimate) There exists a constant  $C_{tt} > 0$  such that

$$\int_0^{T-\tau} \int_{\Omega} \left( \tilde{c}_{h, \bigtriangleup t}(\mathbf{x}, t+\tau) - \tilde{c}_{h, \bigtriangleup t}(\mathbf{x}, t) \right)^2 \mathrm{d}\mathbf{x} \, \mathrm{d}t \le C_{\mathrm{tt}}(\tau + \bigtriangleup t)$$

for all  $\tau \in (0,T)$ .

Proof We set

$$T_T := \int_0^{T-\tau} \int_{\Omega} \left( \tilde{c}_{h, \bigtriangleup t}(\mathbf{x}, t+\tau) - \tilde{c}_{h, \bigtriangleup t}(\mathbf{x}, t) \right)^2 \mathrm{d}\mathbf{x} \, \mathrm{d}t \, .$$

Using the definition of  $\tilde{c}_{h, \Delta t}$  given by (5.5), we can rewrite  $T_T$  as

$$T_T = \int_0^{T-\tau} \sum_{D \in \mathscr{D}_h} |D| \left( c_D^{n_1(t)} - c_D^{n_2(t)} \right)^2 dt \,,$$

where

$$n_1(t) \in \{1, 2, \dots, N\}$$
 is such that  $t_{n_1-1} < t + \tau \le t_{n_1}$ ,  
 $n_2(t) \in \{1, 2, \dots, N\}$  is such that  $t_{n_2-1} < t \le t_{n_2}$ .

We now use (3.6b) and the growth condition imposed on  $\beta$  in Assumption (A1) and estimate

$$\begin{split} T_T &\leq \frac{1}{c_{\beta}} \int_0^{T-\tau} \sum_{D \in \mathscr{D}_h^{int}} |D| \left( c_D^{n_1(t)} - c_D^{n_2(t)} \right) \left( \beta \left( c_D^{n_1(t)} \right) - \beta \left( c_D^{n_2(t)} \right) \right) \mathrm{d}t \\ &= \frac{1}{c_{\beta}} \int_0^{T-\tau} \sum_{D \in \mathscr{D}_h^{int}} |D| \left( c_D^{n_1(t)} - c_D^{n_2(t)} \right) \sum_{n=1}^N \chi(n,t) \left( \beta (c_D^n) - \beta (c_D^{n-1}) \right) \mathrm{d}t \,, \end{split}$$

where the function  $\chi(n,t)$  is defined as

$$\chi(n,t) := \begin{cases} 1 & \text{if } t \le t_{n-1} < t + \tau \\ 0 & \text{otherwise} \end{cases}$$

In view of the definition (3.6a)–(3.6c) of the combined scheme and of Corollary 4.1, we have

$$T_{T} \leq \frac{1}{c_{\beta}} \sum_{n=1}^{N} \triangle t_{n} \int_{0}^{T-\tau} \chi(n,t) \sum_{D \in \mathscr{D}_{h}^{int}} \left( c_{D}^{n_{1}(t)} - c_{D}^{n_{2}(t)} \right) \left( \sum_{E \in \mathscr{N}(D)} \mathbb{S}_{D,E}^{n}(c_{E}^{n} - c_{D}^{n}) - \sum_{E \in \mathscr{N}(D)} v_{D,E}^{n} \overline{c_{D,E}^{n}} - F(c_{D}^{n}) |D| + q_{D}^{n} |D| \right) dt.$$
(5.6)

We now estimate each term separately.

Diffusion term

We set

$$T_D := \sum_{n=1}^N \triangle t_n \int_0^{T-\tau} \chi(n,t) \sum_{D \in \mathscr{D}_h} \left( c_D^{n_1(t)} - c_D^{n_2(t)} \right) \sum_{E \in \mathscr{N}(D)} \mathbb{S}_{D,E}^n(c_E^n - c_D^n) \, \mathrm{d}t \,,$$

where we have changed the summation over  $D \in \mathcal{D}_h^{int}$  into the summation over  $D \in \mathcal{D}_h$  using (3.6b). This enables us to rewrite  $T_D$  as a summation over interior dual sides, since each  $\sigma_{D,E} \in \mathcal{F}_h^{int}$  is in the original sum just twice. This gives

$$T_{D} = \sum_{n=1}^{N} \triangle t_{n} \int_{0}^{T-\tau} \chi(n,t) \sum_{\sigma_{D,E} \in \mathscr{F}_{h}^{\text{int}}} \mathbb{S}_{D,E}^{n} \Big[ (c_{E}^{n} - c_{D}^{n}) \Big( c_{D}^{n_{1}(t)} - c_{E}^{n_{1}(t)} \Big) \\ + (c_{E}^{n} - c_{D}^{n}) \Big( c_{E}^{n_{2}(t)} - c_{D}^{n_{2}(t)} \Big) \Big] dt \,.$$

Using the inequality  $cab \le |c|a^2/2 + |c|b^2/2$  and the estimate (4.2) on  $|\mathbb{S}_{D,E}^n|$ , we can write

$$T_D \le T_{D_1} + T_{D_2} + T_{D_3}$$

with

$$\begin{split} T_{D_1} &:= C_{\mathbf{S},d,\mathscr{T}} \sum_{n=1}^N \bigtriangleup t_n \int_0^{T-\tau} \chi(n,t) \sum_{\sigma_{D,E} \in \mathscr{F}_h^{\text{int}}} \operatorname{diam}(K_{D,E})^{d-2} (c_E^n - c_D^n)^2 \, \mathrm{d}t \,, \\ T_{D_2} &:= \frac{C_{\mathbf{S},d,\mathscr{T}}}{2} \sum_{n=1}^N \bigtriangleup t_n \int_0^{T-\tau} \chi(n,t) \sum_{\sigma_{D,E} \in \mathscr{F}_h^{\text{int}}} \operatorname{diam}(K_{D,E})^{d-2} \left( c_E^{n_1(t)} - c_D^{n_1(t)} \right)^2 \, \mathrm{d}t \,, \\ T_{D_3} &:= \frac{C_{\mathbf{S},d,\mathscr{T}}}{2} \sum_{n=1}^N \bigtriangleup t_n \int_0^{T-\tau} \chi(n,t) \sum_{\sigma_{D,E} \in \mathscr{F}_h^{\text{int}}} \operatorname{diam}(K_{D,E})^{d-2} \left( c_E^{n_2(t)} - c_D^{n_2(t)} \right)^2 \, \mathrm{d}t \,, \end{split}$$

where  $C_{\mathbf{S},d,\mathscr{T}} := \frac{C_{\mathbf{S}}}{\kappa_{\mathscr{T}}} \frac{1}{(d-1)^2}$ .

We now notice that

$$\int_0^{T-\tau} \chi(n,t) \,\mathrm{d}t \le \tau \,, \tag{5.7}$$

since the function  $\chi(n,t)$ , for fixed *n*, is nonzero and equal to one just on the interval  $(t_{n-1} - \tau, t_{n-1}]$  of length  $\tau$ . Using this and the a priori estimate (5.3), we have

$$T_{X_1}^* := \sum_{n=1}^N \triangle t_n \|c_h^n\|_{X_h}^2 \int_0^{T-\tau} \chi(n,t) \, \mathrm{d}t \le \tau \frac{C_{\mathrm{ae}}}{c_{\mathbf{S}}} \,. \tag{5.8}$$

We now introduce a term  $T_{X_3}^*$ ,

$$T_{X_3}^* := \sum_{n=1}^N \triangle t_n \int_0^{T-\tau} \chi(n,t) \, \|c_h^{n_2(t)}\|_{X_h}^2 \, \mathrm{d}t$$

and have, using the definition of  $n_2(t)$ ,

$$T_{X_3}^* = \sum_{n=1}^N \triangle t_n \sum_{m=1}^N \int_{t_{m-1}}^{t_m} \chi(n,t) \|c_h^{n_2(t)}\|_{X_h}^2 dt = \sum_{m=1}^N \|c_h^m\|_{X_h}^2 \sum_{n=1}^N \triangle t_n \int_{t_{m-1}}^{t_m} \chi(n,t) dt.$$
(5.9)

Let us now consider the case where the time step is constant, i.e.  $\triangle t_n = \triangle t$  for all  $n \in \{1, 2, ..., N\}$ . We then have, using a simple change of variables and the fact that  $t_{m-1} - t_{n-1} = t_m - t_n$ ,

$$\sum_{n=1}^{N} \triangle t_n \int_{t_{m-1}}^{t_m} \chi(n,t) \, \mathrm{d}t = \sum_{n=1}^{N} \triangle t \int_{t_{m-1}-t_{n-1}}^{t_m-t_{n-1}} \chi(n,s+t_{n-1}) \, \mathrm{d}s$$
$$= \triangle t \sum_{n=1}^{N} \int_{t_m-t_n}^{t_m-t_{n-1}} 1_{-\tau < s \le 0} \, \mathrm{d}s \le \tau \triangle t \,,$$

where the function  $1_{a < s \le b}$  is equal to 1 on the interval (a, b] and zero otherwise, which we substitute back into (5.9) and use the a priori estimate (5.3) to obtain

$$T_{X_3}^* \leq \tau \frac{C_{\mathrm{ae}}}{c_{\mathbf{S}}} \,.$$

Next we consider a nonconstant time step. We have

$$\sum_{n=1}^N \triangle t_n \chi(n,t) \leq \tau + \triangle t \,,$$

considering that  $\chi(n,t)$ , for fixed *t*, is nonzero and equal to one just when  $t \leq t_{n-1} < t + \tau$ , i.e. an interval of length  $\tau$ , and that with each such *n*, we add  $\Delta t_n$ . Using this, we have

$$T_{X_3}^* \leq (\tau + \triangle t) \sum_{m=1}^N \|c_h^m\|_{X_h}^2 \triangle t_m \leq (\tau + \triangle t) \frac{C_{\mathrm{ae}}}{c_{\mathbf{S}}}.$$

We next introduce a term  $T_{X_2}^*$ ,

$$T_{X_2}^* := \sum_{n=1}^N \triangle t_n \int_0^{T-\tau} \chi(n,t) \, \|c_h^{n_1(t)}\|_{X_h}^2 \, \mathrm{d}t \, .$$

Similarly as in the previous case, using the definition of  $n_1(t)$ , we have

$$T_{X_2}^* \leq \sum_{n=1}^N \triangle t_n \sum_{m=1}^N \int_{t_{m-1}-\tau}^{t_m-\tau} \chi(n,t) \|c_h^{n_1(t)}\|_{X_h}^2 dt$$
  
=  $\sum_{m=1}^N \|c_h^m\|_{X_h}^2 \sum_{n=1}^N \triangle t_n \int_{t_{m-1}-\tau}^{t_m-\tau} \chi(n,t) dt$ ,

which yields the same estimate for  $T^*_{X_2}$  as for  $T^*_{X_3}$ . We finally introduce

$$T_{L_{1}}^{*} := \sum_{n=1}^{N} \triangle t_{n} \sum_{D \in \mathscr{D}_{h}} (c_{D}^{n})^{2} |D| \int_{0}^{T-\tau} \chi(n,t) \, \mathrm{d}t \le \tau T \frac{C_{\mathrm{ae}}}{c_{\beta}}, \qquad (5.10)$$

which we have estimated using (5.7) and the a priori estimate (5.1), and

$$T_{L_{i}}^{*} := \sum_{n=1}^{N} \triangle t_{n} \int_{0}^{T-\tau} \chi(n,t) \sum_{D \in \mathscr{D}_{h}} \left( c_{D}^{n_{i-1}(t)} \right)^{2} |D| \, \mathrm{d}t \qquad i \in \{2,3\}.$$

We shall need  $T_{L_i}^*$ ,  $i \in \{1, 2, 3\}$ , for the estimates of the other terms of  $T_T$  below. Using the a priori estimate (5.1) and the same techniques as for  $T_{X_i}^*$ , i = 2, 3, we altogether come to

$$T_{X_i}^* \le \tau \frac{C_{\mathrm{ae}}}{c_{\mathbf{S}}}, \quad T_{L_i}^* \le \tau T \frac{C_{\mathrm{ae}}}{c_{\beta}} \qquad i \in \{2,3\}$$
(5.11)

for a constant time step and

$$T_{X_i}^* \le (\tau + \triangle t) \frac{C_{ae}}{c_{\mathbf{S}}}, \quad T_{L_i}^* \le (\tau + \triangle t) T \frac{C_{ae}}{c_{\beta}} \qquad i \in \{2, 3\}$$
(5.12)

for a generally nonconstant time step. Now using (3.3) for  $T_{D_1}$ ,  $T_{D_2}$ , and  $T_{D_3}$ , we have

$$T_D \le \frac{C_{\mathbf{S}}}{\kappa_{\mathscr{T}}^2} \frac{d+1}{2d(d-1)^2} \left( T_{X_1}^* + \frac{1}{2} T_{X_2}^* + \frac{1}{2} T_{X_3}^* \right).$$
(5.13)

## Convection term

We will write the convection term as  $T_{C_1} + T_{C_2}$ , with

$$T_{C_1} := -\sum_{n=1}^{N} \triangle t_n \int_0^{T-\tau} \chi(n,t) \sum_{D \in \mathscr{D}_h} \left( c_D^{n_1(t)} - c_D^{n_2(t)} \right) \sum_{E \in \mathscr{N}(D)} v_{D,E}^n \widehat{c_{D,E}^n} \, \mathrm{d}t$$

and

$$T_{C_2} := -\sum_{n=1}^{N} \triangle t_n \int_0^{T-\tau} \chi(n,t) \sum_{D \in \mathscr{D}_h} \left( c_D^{n_1(t)} - c_D^{n_2(t)} \right) \sum_{E \in \mathscr{N}(D)} |v_{D,E}^n| \; \alpha_{D,E}^n(c_E^n - c_D^n) \; \mathrm{d}t \,,$$

using the splitting into full upstream weighting and coefficient-centered weighting.

We again rewrite  $T_{C_1}$  as the summation over the interior dual sides; we however adjust the denotation of the dual volumes sharing a given side  $\sigma_{D,E}$  such that  $v_{D,E}^n \ge 0$ . Then, using the definition of the upstream weighting,  $T_{C_1}$  writes

$$\sum_{n=1}^{N} \triangle t_n \int_0^{T-\tau} \chi(n,t) \sum_{\sigma_{D,E} \in \mathscr{F}_h^{\text{int}}, v_{D,E}^n \ge 0} -v_{D,E}^n c_D^n \left( c_D^{n_1(t)} - c_E^{n_1(t)} + c_E^{n_2(t)} - c_D^{n_2(t)} \right) \mathrm{d}t \,.$$

Using  $\pm ab \leq \varepsilon a^2/2 + b^2/(2\varepsilon)$ ,  $\varepsilon > 0$ , where we put  $\varepsilon = d_{D,E}$ , we come to

$$T_{C_1} \le T_{C_3} + T_{C_4} + T_{C_5}$$

with

$$\begin{split} T_{C_3} &:= \sum_{n=1}^N \triangle t_n \int_0^{T-\tau} \chi(n,t) \sum_{\substack{\sigma_{D,E} \in \mathscr{F}_h^{\text{int}}, v_{D,E}^n \ge 0 \\ \sigma_{D,E} \in \mathscr{F}_h^{\text{int}}, v_{D,E}^n \ge 0 }} |v_{D,E}^n | d_{D,E} (c_D^n)^2 \, \mathrm{d}t \,, \\ T_{C_4} &:= \frac{1}{2} \sum_{n=1}^N \triangle t_n \int_0^{T-\tau} \chi(n,t) \sum_{\substack{\sigma_{D,E} \in \mathscr{F}_h^{\text{int}} \\ \sigma_{D,E} \in \mathscr{F}_h^{\text{int}}}} \frac{|v_{D,E}^n|}{d_{D,E}} \left( c_E^{n_1(t)} - c_D^{n_1(t)} \right)^2 \, \mathrm{d}t \,, \\ T_{C_5} &:= \frac{1}{2} \sum_{n=1}^N \triangle t_n \int_0^{T-\tau} \chi(n,t) \sum_{\substack{\sigma_{D,E} \in \mathscr{F}_h^{\text{int}} \\ \sigma_{D,E} \in \mathscr{F}_h^{\text{int}}}} \frac{|v_{D,E}^n|}{d_{D,E}} \left( c_E^{n_2(t)} - c_D^{n_2(t)} \right)^2 \, \mathrm{d}t \,. \end{split}$$

We have

$$\begin{split} \sum_{\substack{\sigma_{D,E}\in\mathscr{F}_{h}^{\text{int}}, v_{D,E}^{n}\geq 0 \\ \leq \frac{C_{\mathbf{v}}}{\kappa_{\mathscr{T}}}\frac{d+1}{d-1}\sum_{D\in\mathscr{D}_{h}}\left(\frac{|K_{D}|}{d+1}+\frac{|L_{D}|}{d+1}\right)(c_{D}^{n})^{2} = \frac{C_{\mathbf{v}}}{\kappa_{\mathscr{T}}}\frac{d+1}{d-1}\sum_{D\in\mathscr{D}_{h}}(c_{D}^{n})^{2}|D|, \end{split}$$

where we have used Assumption (A4), which implies  $|v_{D,E}^n| \leq C_v |\sigma_{D,E}|$ , (3.5), Assumption (B), (3.6b), the fact that each dual volume  $D \in \mathcal{D}_h^{int}$  has *d* dual sides

inside a simplex  $K_D$  and d dual sides inside a simplex  $L_D$  and that  $c_D^n$  can appear as an upwind value only at these sides, and (3.2). Thus, we have

$$T_{C_3} \leq \frac{C_{\mathbf{v}}}{\kappa_{\mathscr{T}}} \frac{d+1}{d-1} T_{L_1}^* \,.$$

Using  $|v_{D,E}^n| \leq C_{\mathbf{v}} |\sigma_{D,E}|$  and (3.4), we have

$$T_{C_i} \leq \frac{C_{\mathbf{v}}}{\kappa_{\mathscr{T}}} \frac{d+1}{4(d-1)} T^*_{X_{i-2}} \qquad i \in \{4,5\},$$

which altogether leads to

$$T_{C_1} \le \frac{C_{\mathbf{v}}}{\kappa_{\mathscr{T}}} \left( \frac{d+1}{d-1} T_{L_1}^* + \frac{d+1}{4(d-1)} (T_{X_2}^* + T_{X_3}^*) \right).$$
(5.14)

We now consider  $T_{C_2}$ . We can easily notice that it is almost same as the diffusion term  $T_D$ , except for the term  $\mathbb{S}_{D,E}^n$ , which is replaced by  $|v_{D,E}^n| \alpha_{D,E}^n$ . Using  $|v_{D,E}^n| \le C_{\mathbf{v}} |\sigma_{D,E}|$ ,  $\alpha_{D,E}^n \le 1/2$ , and the estimates (3.3) and (3.5), we easily come to

$$T_{C_2} \le \frac{C_{\mathbf{v}}}{\kappa_{\mathscr{T}}} h \frac{d+1}{4d(d-1)} \left( T_{X_1}^* + \frac{1}{2} T_{X_2}^* + \frac{1}{2} T_{X_3}^* \right).$$
(5.15)

Reaction term

We denote

$$T_R := -\sum_{n=1}^N \triangle t_n \int_0^{T-\tau} \chi(n,t) \sum_{D \in \mathscr{D}_h} \left( c_D^{n_1(t)} - c_D^{n_2(t)} \right) F(c_D^n) |D| \, \mathrm{d}t \, .$$

We estimate

$$-F(c_D^n)(c_D^{n_1}-c_D^{n_2}) \le \frac{(c_D^{n_1}-c_D^{n_2})^2}{2} + \frac{(F(c_D^n))^2}{2} \le (c_D^{n_1})^2 + (c_D^{n_2})^2 + \frac{L_F^2(c_D^n)^2}{2},$$

using the inequalities  $ab \le a^2/2 + b^2/2$ ,  $(a-b)^2/2 \le a^2 + b^2$ , the Lipschitz continuity of *F* with the constant  $L_F$ , and the fact that F(0) = 0, following either from Assumption (A5) or (A6). This implies

$$T_R \le \left(\frac{L_F^2}{2}T_{L_1}^* + T_{L_2}^* + T_{L_3}^*\right).$$
(5.16)

Sources term

We denote

$$T_{S} := \sum_{n=1}^{N} \triangle t_{n} \int_{0}^{T-\tau} \chi(n,t) \sum_{D \in \mathscr{D}_{h}} \left( c_{D}^{n_{1}(t)} - c_{D}^{n_{2}(t)} \right) q_{D}^{n} |D| \, \mathrm{d}t.$$

Using the same estimate as for the reaction term, (5.7), and (4.5), we come to

$$T_{S} \leq \frac{1}{2}\tau \|q\|_{0,Q_{T}}^{2} + T_{L_{2}}^{*} + T_{L_{3}}^{*}.$$
(5.17)

The proof of the lemma is concluded by introducing (5.13), (5.14), (5.15), (5.16), and (5.17) into (5.6), while using the estimates (5.8), (5.10), and (5.12).

*Remark 5.2 (Time translate estimate under Assumption (D))* If Assumption (D) is valid, the transmissibilities  $\mathbb{S}_{D,E}^n$  are non-negative as in the finite volume method. Hence  $T_D \leq T_{D_1} + T_{D_2} + T_{D_3}$  with

$$T_{D_1} = \sum_{n=1}^N \triangle t_n \int_0^{T-\tau} \chi(n,t) \sum_{\sigma_{D,E} \in \mathscr{F}_h^{\text{int}}} \mathbb{S}_{D,E}^n (c_E^n - c_D^n)^2 dt$$

and similarly for  $T_{D_2}$  and  $T_{D_3}$ . Thus using

$$\sum_{\sigma_{D,E}\in\mathscr{F}_{h}^{\text{int}}} \mathbb{S}_{D,E}^{n} (c_{E}^{n} - c_{D}^{n})^{2} = -\sum_{D\in\mathscr{D}_{h}} c_{D} \sum_{E\in\mathscr{D}_{h}} \mathbb{S}_{D,E}^{n} c_{E}$$

and (4.1),  $T_D \leq C_{\mathbf{S}}(T_{X_1}^* + T_{X_2}^*/2 + T_{X_3}^*/2)$  in this case instead of (5.13).

*Remark 5.3 (Time translate estimate for a constant time step)* For a constant time step, we have indeed an  $O(\tau)$  estimate, using (5.11) instead of (5.12).

We give below a space translate estimate for  $\tilde{c}_{h,\Delta t}$  given by (5.5). It extends the estimate from [26,27] to the case of (dual) meshes not necessarily satisfying the orthogonality property; we only need the shape regularity Assumption (B) and the constant  $C_{\rm st}$  only depends on d,  $\kappa_{\mathcal{T}}$ , and  $C_{\rm ae}/c_{\rm S}$ . The proof is analogous to that of [42, Theorem 3.5], uses the a priori estimate (5.3), and can be found in [41].

**Lemma 5.3 (Space translate estimate)** *Let us define*  $\tilde{c}_{h, \triangle t}(\mathbf{x}, t)$  *by zero outside of*  $\Omega$ *. Then there exists a constant*  $C_{st} > 0$  *such that* 

$$\int_0^T \int_{\Omega} \left( \tilde{c}_{h, \triangle t} (\mathbf{x} + \boldsymbol{\xi}, t) - \tilde{c}_{h, \triangle t} (\mathbf{x}, t) \right)^2 \mathrm{d}\mathbf{x} \, \mathrm{d}t \le C_{\mathrm{st}} |\boldsymbol{\xi}| (|\boldsymbol{\xi}| + h)$$

for all  $\xi \in \mathbb{R}^d$ .

## **6** Convergence

Using the a priori estimates of the previous section and the Kolmogorov relative compactness theorem, we show in this section that the approximate solutions converge strongly in  $L^2(Q_T)$  to a function *c* and we prove that *c* is a weak solution of the continuous problem.

6.1 Strong convergence in  $L^2(Q_T)$ 

**Theorem 6.1 (Strong convergence in**  $L^2(Q_T)$ ) There exist subsequences of  $\tilde{c}_{h, \Delta t}$ and  $c_{h, \Delta t}$  which converge strongly in  $L^2(Q_T)$  to a function  $c \in L^2(0, T; H_0^1(\Omega))$ .

*Proof* Let us consider the sequence  $\tilde{c}_{h,\Delta t}$ . The a priori estimate (5.1) and Lemmas 5.2 and 5.3 imply that  $\tilde{c}_{h,\Delta t}$  satisfies the assumptions of Lemma 8.4 in Appendix 8. Thus  $\tilde{c}_{h,\Delta t}$  verifies the assumptions of the Kolmogorov theorem ([11, Theorem IV.25], [23, Theorem 14.1]) and consequently is relatively compact in  $L^2(Q_T)$ . This implies the existence of a subsequence of  $\tilde{c}_{h,\Delta t}$  which converges strongly to some function c in  $L^2(Q_T)$ . Moreover, due to the space translate estimate of Lemma 5.3, [23, Theorem 14.2] gives that  $c \in L^2(0,T;H_0^1(\Omega))$ . Finally, considering Lemma 5.1,  $c_{h,\Delta t}$  converges to the same c.  $\Box$ 

*Remark 6.1 (Relative compactness for a constant time step)* Using Remark 5.3, the a priori estimate (5.1) and Lemmas 5.2 and 5.3 directly imply that  $\tilde{c}_{h,\Delta t}$  verifies the assumptions of the Kolmogorov theorem for a constant time step. Hence, in this case Lemma 8.4 is not necessary.

#### 6.2 Convergence to a weak solution

We have shown in Theorem 6.1 that subsequences of  $\tilde{c}_{h,\triangle t}$  and  $c_{h,\triangle t}$ , which we still denote by  $\tilde{c}_{h,\triangle t}$  and  $c_{h,\triangle t}$ , converge strongly in  $L^2(Q_T)$  to some function  $c \in L^2(0,T;H_0^1(\Omega))$ . We now show that c is a weak solution of the continuous problem. For this purpose, we introduce

$$\Psi := \left\{ \psi \in C^{2,1}(\overline{\Omega} \times [0,T]), \, \psi = 0 \text{ on } \partial \Omega \times [0,T], \, \psi(\cdot,T) = 0 \right\}.$$
(6.1)

We then take an arbitrary  $\psi \in \Psi$ , multiply (3.6c) by  $\triangle t_n \psi(Q_D, t_{n-1})$ , and sum the result over  $D \in \mathcal{D}_h^{int}$  and n = 1, ..., N. This gives

$$T_T + T_D + T_C + T_R = T_S \tag{6.2}$$

with

$$\begin{split} T_T &:= \sum_{n=1}^N \sum_{D \in \mathscr{D}_h} \left( \beta(c_D^n) - \beta(c_D^{n-1}) \right) \psi(Q_D, t_{n-1}) |D|, \\ T_D &:= \sum_{n=1}^N \bigtriangleup t_n \sum_{D \in \mathscr{D}_h} \sum_{E \in \mathscr{D}_h} c_E^n \sum_{K \in \mathscr{T}_h} (\mathbf{S}^n \nabla \varphi_E, \nabla \varphi_D)_{0,K} \psi(Q_D, t_{n-1}), \\ T_C &:= \sum_{n=1}^N \bigtriangleup t_n \sum_{D \in \mathscr{D}_h} \sum_{E \in \mathscr{N}(D)} v_{D,E}^n \overline{c_{D,E}^n} \psi(Q_D, t_{n-1}), \\ T_R &:= \sum_{n=1}^N \bigtriangleup t_n \sum_{D \in \mathscr{D}_h} F(c_D^n) \psi(Q_D, t_{n-1}) |D|, \\ T_S &:= \sum_{n=1}^N \bigtriangleup t_n \sum_{D \in \mathscr{D}_h} q_D^n \psi(Q_D, t_{n-1}) |D|, \end{split}$$

using  $\psi(Q_D, t_{n-1}) = 0$  for all  $D \in \mathscr{D}_h^{ext}$  and n = 1, ..., N. We now show that each of the above terms converges to its continuous version as h and  $\Delta t$  tend to zero.

## Time evolution term

We use the discrete integration by parts formula and the fact that  $\psi(Q_D, t_N) = 0$  for all  $D \in \mathcal{D}_h$  to obtain

$$T_{T} = -\sum_{n=1}^{N} \sum_{D \in \mathscr{D}_{h}} \beta(c_{D}^{n}) \Big( \Psi(Q_{D}, t_{n}) - \Psi(Q_{D}, t_{n-1}) \Big) |D| - \sum_{D \in \mathscr{D}_{h}} \beta(c_{D}^{0}) \Psi(Q_{D}, 0) |D|.$$
(6.3)

We would now like to show that

$$\sum_{D \in \mathscr{D}_h} \beta(c_D^0) \psi(Q_D, 0) |D| \longrightarrow \int_{\Omega} \beta(c_0(\mathbf{x})) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} \text{ as } h \to 0.$$
(6.4)

For this purpose, we introduce

$$T_{T_1} := \sum_{D \in \mathscr{D}_h} \int_D \left( \beta(c_D^0) \psi(Q_D, 0) - \beta(c_0(\mathbf{x})) \psi(\mathbf{x}, 0) \right) d\mathbf{x}$$

We add and subtract  $\beta(c_D^0)\psi(\mathbf{x},0)$  to each term and rewrite  $T_{T_1}$  as

$$\sum_{D \in \mathscr{D}_h} \int_D \beta(c_D^0) \Big( \psi(Q_D, 0) - \psi(\mathbf{x}, 0) \Big) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_0(\mathbf{x})) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_D^0) - \beta(c_D^0) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_D^0) - \beta(c_D^0) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_D^0) - \beta(c_D^0) - \beta(c_D^0) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \int_D \Big( \beta(c_D^0) - \beta(c_D^0) - \beta(c_D^0) - \beta(c_D^0) \Big) \psi(\mathbf{x}, 0) \, \mathrm{d}\mathbf{x} + \sum_{D \in \mathscr{D}_h} \Big( \beta(c_D^0) - \beta(c$$

Using the definition of  $c_D^0$  given by (3.6a) for  $D \in \mathscr{D}_h^{int}$  and by (3.6b) for  $D \in \mathscr{D}_h^{ext}$ , the fact that  $\beta$  is increasing by Assumption (A1), and Assumption (A8), we have that  $|\beta(c_D^0)| \leq \beta(M)$  for all  $D \in \mathscr{D}_h$ . Due to the boundedness of  $|\Psi|$  by  $C_{1,\Psi}$ , we can bound  $|T_{T_1}|$  by

$$\beta(M)\sum_{D\in\mathscr{D}_h}\int_D |\psi(Q_D,0)-\psi(\mathbf{x},0)|\,\mathrm{d}\mathbf{x}+C_{1,\psi}\sum_{D\in\mathscr{D}_h}\int_D |\beta(c_D^0)-\beta(c_0(\mathbf{x}))|\,\mathrm{d}\mathbf{x}.$$

Since  $\psi \in C^{2,1}(\overline{\Omega} \times [0,T])$ , we have

$$|\boldsymbol{\psi}(\boldsymbol{Q}_D, \boldsymbol{0}) - \boldsymbol{\psi}(\mathbf{x}, \boldsymbol{0})| \leq C_{2, \boldsymbol{\psi}} |\boldsymbol{Q}_D - \mathbf{x}| \leq C_{2, \boldsymbol{\psi}} h$$

for all  $\mathbf{x} \in D$ , and thus the first term of the bound for  $|T_{T_1}|$  tends to 0 as  $h \to 0$ . We now consider its second term. We have, for boundary dual volumes,

$$\sum_{D \in \mathscr{D}_h^{ext}} \int_D |c_D^0 - c_0(\mathbf{x})| \, \mathrm{d} \mathbf{x} \le M \sum_{D \in \mathscr{D}_h^{ext}} |D| \le M |\partial \Omega| h \,,$$

using (3.6b) and Assumption (A8). Considering in addition the definition of  $\tilde{c}_{h,\triangle t}$ by (5.5) and (3.6a) for interior dual volumes,  $\tilde{c}_{h,\triangle t}(\mathbf{x},0)$  converges to  $c_0(\mathbf{x})$  in  $\Omega$  in the  $L^1$  sense as  $h \to 0$ . Hence at least a subsequence of  $\tilde{c}_{h,\triangle t}(\mathbf{x},0)$ , which we still denote by  $\tilde{c}_{h,\triangle t}(\mathbf{x},0)$ , converges to  $c_0(\mathbf{x})$  pointwise a.e. in  $\Omega$ . Thus also  $\beta(\tilde{c}_{h,\triangle t}(\mathbf{x},0)) \to \beta(c_0(\mathbf{x}))$  a.e. in  $\Omega$ , using the continuity of  $\beta$ . Further, using that  $\beta$  is increasing from Assumption (A1), we have  $|\beta(\tilde{c}_{h, \triangle t}(\mathbf{x}, 0))| \leq \beta(M)$ . Hence the Lebesgue dominated convergence theorem implies

$$\sum_{D \in \mathscr{D}_h} \int_D |\beta(c_D^0) - \beta(c_0(\mathbf{x}))| \, \mathrm{d}\mathbf{x} = \int_\Omega |\beta(\tilde{c}_{h, \triangle t}(\mathbf{x}, 0)) - \beta(c_0(\mathbf{x}))| \, \mathrm{d}\mathbf{x} \longrightarrow 0 \text{ as } h \longrightarrow 0$$

which can be by repetition extended onto whole  $\tilde{c}_{h, \triangle t}(\mathbf{x}, 0)$ . Thus  $T_{T_1} \rightarrow 0$  as  $h \rightarrow 0$  and consequently (6.4) is fulfilled.

Now we intend to prove that

$$\sum_{n=1}^{N} \sum_{D \in \mathscr{D}_{h}} \beta(c_{D}^{n}) \Big( \Psi(\mathcal{Q}_{D}, t_{n}) - \Psi(\mathcal{Q}_{D}, t_{n-1}) \Big) |D| \longrightarrow \int_{0}^{T} \int_{\Omega} \beta(c(\mathbf{x}, t)) \psi_{t}(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t$$
(6.5)

as  $h, \triangle t \rightarrow 0$ . We set

$$T_{T_2} := \sum_{n=1}^N \sum_{D \in \mathscr{D}_h} \Big[ \beta(c_D^n) \Big( \psi(Q_D, t_n) - \psi(Q_D, t_{n-1}) \Big) |D| \\ - \int_{t_{n-1}}^{t_n} \int_D \beta(c(\mathbf{x}, t)) \psi_t(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \Big].$$

We add and subtract  $\int_{t_{n-1}}^{t_n} \int_D \beta(c_D^n) \psi_t(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t$  in each term of  $T_{T_2}$  to obtain

$$T_{T_2} = \sum_{n=1}^{N} \sum_{D \in \mathscr{D}_h} \beta(c_D^n) \int_{t_{n-1}}^{t_n} \int_D \left( \frac{\partial \psi}{\partial t}(Q_D, t) - \frac{\partial \psi}{\partial t}(\mathbf{x}, t) \right) d\mathbf{x} dt \qquad (6.6)$$
$$+ \int_0^T \int_\Omega \left( \beta(\tilde{c}_{h, \bigtriangleup t}(\mathbf{x}, t)) - \beta(c(\mathbf{x}, t)) \right) \psi_t(\mathbf{x}, t) d\mathbf{x} dt .$$

We have, for all  $\mathbf{x} \in D$ , for all  $D \in \mathcal{D}_h$ , and all h > 0,

$$\left|\frac{\partial \psi}{\partial t}(Q_D,t)-\frac{\partial \psi}{\partial t}(\mathbf{x},t)\right|\leq f(h),$$

where the function f satisfies f(h) > 0 and  $f(h) \to 0$  as  $h \to 0$ . This follows by the fact that  $\partial \psi / \partial t \in C(\overline{\Omega})$  from (6.1) and hence is uniformly continuous on  $\overline{\Omega}$ . Thus the first term of (6.6) is bounded by

$$\begin{split} f(h) \sum_{n=1}^{N} \sum_{D \in \mathscr{D}_{h}} |\beta(c_{D}^{n})| \triangle t_{n} |D| &\leq f(h) T^{\frac{1}{2}} |\Omega|^{\frac{1}{2}} \Big( \sum_{n=1}^{N} \sum_{D \in \mathscr{D}_{h}} (\beta(c_{D}^{n}))^{2} \triangle t_{n} |D| \Big)^{\frac{1}{2}} \\ &\leq f(h) T |\Omega|^{\frac{1}{2}} C_{ac\beta}^{\frac{1}{2}}, \end{split}$$

using the Cauchy–Schwarz inequality and the a priori estimate (5.2). Further,  $|\psi_t(\mathbf{x},t)| \leq C_{4,\psi}$ , and thus we can estimate  $T_{T_2}$  by

$$|T_{T_2}| \leq f(h)T|\Omega|^{\frac{1}{2}} C_{\mathrm{ae}\beta}^{\frac{1}{2}} + C_{4,\psi} \int_0^T \int_\Omega |\beta(\tilde{c}_{h,\triangle t}(\mathbf{x},t)) - \beta(c(\mathbf{x},t))| \,\mathrm{d}\mathbf{x}\,\mathrm{d}t.$$
(6.7)

We now use that  $\tilde{c}_{h, \triangle t} \to c$  strongly in  $L^2(Q_T)$  as  $h, \triangle t \to 0$ , due to Theorem 6.1. There exists at least a subsequence of  $\tilde{c}_{h, \triangle t}$ , which we still denote  $\tilde{c}_{h, \triangle t}$ , such that  $\tilde{c}_{h, \triangle t}(\mathbf{x}, t) \to c(\mathbf{x}, t)$  a.e. in  $Q_T$ . Thus, using the continuity of  $\beta(\cdot), \beta(\tilde{c}_{h, \triangle t}(\mathbf{x}, t)) \to \beta(c(\mathbf{x}, t))$  a.e. in  $Q_T$ . Now under Assumption (D), which implies the discrete maximum principle by Theorem 4.5, and using that  $\beta$  is increasing,  $|\beta(\tilde{c}_{h, \triangle t}(\mathbf{x}, t))| \leq \beta(M)$ , and thus we can use the Lebesgue dominated convergence theorem to conclude the convergence of the second term of (6.7) and thus of (6.7) to 0 as  $h, \Delta t \to 0$ . In this case Assumption (A1) suffices.

In the general case we use Assumption (A2). We decompose the function  $\beta$  as  $\beta_1 + \beta_2$ ,

$$\begin{split} \beta_1(s) &:= \beta(s) \ \text{on} \ [-P,P] \,, \quad \beta_1(s) := 0 \ \text{on} \ (-\infty,-P) \cup (P,+\infty) \,, \\ \beta_2(s) &:= 0 \ \text{on} \ [-P,P] \,, \quad \beta_2(s) := \beta(s) \ \text{on} \ (-\infty,-P) \cup (P,+\infty) \,. \end{split}$$

We further introduce a function *y* linearly connecting the points  $[-P, \beta(-P)]$  and  $[P, \beta(P)]$  and zero otherwise,

$$y(s) := \frac{\beta(P) - \beta(-P)}{2P} s + \frac{\beta(P) + \beta(-P)}{2} \text{ on } [-P,P],$$
  
$$y(s) := 0 \text{ on } (-\infty, -P) \cup (P, +\infty).$$

We finally define  $\tilde{\beta}_1 := \beta_1 - y$  and  $\tilde{\beta}_2 := \beta_2 + y$  and remark that  $\beta = \tilde{\beta}_1 + \tilde{\beta}_2$ . Clearly,  $\tilde{\beta}_1$  is continuous on  $\mathbb{R}$  and satisfies  $|\tilde{\beta}_1(s)| \le 2C_\beta$  on  $\mathbb{R}$  and  $\tilde{\beta}_2$  is Lipschitzcontinuous on  $\mathbb{R}$  with max  $\{L_\beta, [\beta(P) - \beta(-P)]/(2P)\}$ . We now estimate

$$\begin{split} &\int_0^T \int_{\Omega} |\boldsymbol{\beta}(\tilde{c}_{h,\triangle t}(\mathbf{x},t)) - \boldsymbol{\beta}(c(\mathbf{x},t))| \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \leq \int_0^T \int_{\Omega} |\tilde{\beta}_1(\tilde{c}_{h,\triangle t}(\mathbf{x},t))| \\ &- \tilde{\beta}_1(c(\mathbf{x},t))| \, \mathrm{d}\mathbf{x} \, \mathrm{d}t + \int_0^T \int_{\Omega} |\tilde{\beta}_2(\tilde{c}_{h,\triangle t}(\mathbf{x},t)) - \tilde{\beta}_2(c(\mathbf{x},t))| \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \, . \end{split}$$

The first term of the above expression converges to zero using the Lebesgue dominated convergence theorem as in the previous case. For the second term, it suffices to use the Lipschitz continuity of  $\tilde{\beta}_2$  and the strong convergence of  $\tilde{c}_{h, \Delta t}$  to *c* in  $L^2(Q_T)$ . Thus (6.5) is satisfied. Combining (6.4) and (6.5), we have

$$T_T \longrightarrow -\int_0^T \int_{\Omega} \beta(c(\mathbf{x},t)) \psi_t(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t - \int_{\Omega} \beta(c_0(\mathbf{x})) \psi(\mathbf{x},0) \, \mathrm{d}\mathbf{x}$$
(6.8)

as  $h, \triangle t \to 0$ .

Diffusion term

We rewrite  $T_D$  as

$$T_D = \sum_{n=1}^N \triangle t_n \sum_{K \in \mathscr{T}_h} \int_K \mathbf{S}^n \nabla c_h^n(\mathbf{x}) \cdot \nabla \Big( \sum_{D \in \mathscr{D}_h} \psi(Q_D, t_{n-1}) \varphi_D(\mathbf{x}) \Big) \, \mathrm{d}\mathbf{x},$$

using the definition of  $c_h^n \in X_h$ , and define

$$\mathbf{S}_{\Delta t}(\mathbf{x},t) := \mathbf{S}^{n}(\mathbf{x}) \text{ for } \mathbf{x} \in \Omega, t \in (t_{n-1},t_{n}] \qquad n \in \{1,\ldots,N\},$$
(6.9)

where  $S^n$  is given by (3.10) for the nonconforming method and by (3.12) for the mixed-hybrid method. We will show the validity of two passages to the limit. We begin by showing that

$$\sum_{n=1}^{N} \triangle t_n \sum_{K \in \mathscr{T}_h} \int_K \mathbf{S}^n \nabla c_h^n(\mathbf{x}) \cdot \nabla \Big( \sum_{D \in \mathscr{D}_h} \psi(Q_D, t_{n-1}) \varphi_D(\mathbf{x}) \Big) \, \mathrm{d}\mathbf{x}$$
(6.10)  
$$- \sum_{n=1}^{N} \triangle t_n \sum_{K \in \mathscr{T}_h} \int_K \mathbf{S}^n \nabla c_h^n(\mathbf{x}) \cdot \nabla \psi(\mathbf{x}, t_{n-1}) \, \mathrm{d}\mathbf{x} \longrightarrow 0 \text{ as } h \to 0.$$

We set

$$I_{\psi}(\cdot,t_{n-1}):=\sum_{D\in\mathscr{D}_h}\psi(Q_D,t_{n-1})\varphi_D$$

and

$$T_{D_1} := \sum_{n=1}^N \triangle t_n \sum_{K \in \mathscr{T}_h} \int_K \mathbf{S}^n \nabla c_h^n(\mathbf{x}) \cdot \nabla \Big( I_{\Psi}(\mathbf{x}, t_{n-1}) - \Psi(\mathbf{x}, t_{n-1}) \Big) \, \mathrm{d}\mathbf{x} \, .$$

We then estimate

$$|T_{D_1}| \leq C_{\mathbf{S}} \sum_{n=1}^N \triangle t_n \|c_h^n\|_{X_h} \|I_{\Psi}(\cdot, t_{n-1}) - \Psi(\cdot, t_{n-1})\|_{X_h}$$

using the Cauchy-Schwarz inequality. Next we use the interpolation estimate

$$\begin{split} \|I_{\boldsymbol{\psi}}(\cdot,t_{n-1}) - \boldsymbol{\psi}(\cdot,t_{n-1})\|_{X_{h}} &= \Big(\sum_{K\in\mathscr{T}_{h}}\int_{K} \Big|\nabla\big(I_{\boldsymbol{\psi}}(\cdot,t_{n-1}) - \boldsymbol{\psi}(\cdot,t_{n-1})\big)\Big|^{2}\,\mathrm{d}\mathbf{x}\Big)^{\frac{1}{2}} \\ &\leq C_{I}\boldsymbol{\theta}_{\mathscr{T}}h\Big(\sum_{K\in\mathscr{T}_{h}}|\boldsymbol{\psi}(\cdot,t_{n-1})|_{2,K}^{2}\Big)^{\frac{1}{2}} \leq C_{I}\boldsymbol{\theta}_{\mathscr{T}}C_{5,\boldsymbol{\psi}}h, \end{split}$$

where  $\theta_{\mathscr{T}}$  is given by the consequence (3.1) of Assumption (B),  $C_I$  does not depend on h (nor on  $\Delta t$ ), and  $|\cdot|_{2,K}$  denotes the  $H^2$  seminorm, see for instance [17, Theorem 15.3]. Finally, the Cauchy–Schwarz inequality yields

$$|T_{D_1}| \le C_{\mathbf{S}} C_I \theta_{\mathscr{T}} C_{5,\psi} h \Big( \sum_{n=1}^N \triangle t_n \| c_h^n \|_{X_h}^2 \Big)^{\frac{1}{2}} \Big( \sum_{n=1}^N \triangle t_n \Big)^{\frac{1}{2}} = C_{\mathbf{S}} C_I \theta_{\mathscr{T}} C_{5,\psi} T^{\frac{1}{2}} \Big( \frac{C_{ae}}{c_{\mathbf{S}}} \Big)^{\frac{1}{2}} h$$

using the a priori estimate (5.3). Hence (6.10) is fulfilled. We next show that

$$\sum_{n=1}^{N} \triangle t_n \sum_{K \in \mathscr{T}_h} \int_K \mathbf{S}^n \nabla c_h^n(\mathbf{x}) \cdot \nabla \psi(\mathbf{x}, t_{n-1}) \, \mathrm{d}\mathbf{x} \longrightarrow \int_0^T \int_{\Omega} \mathbf{S} \nabla c(\mathbf{x}, t) \cdot \nabla \psi(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t$$
(6.11)

as  $h, \triangle t \to 0$ . We see that both  $c_h^n(\mathbf{x})$  and  $\psi(\mathbf{x}, t_{n-1})$  are constant in time, so that we can easily introduce an integral with respect to time into the first term of (6.11). We further add and subtract  $\sum_{n=1}^{N} \int_{t_{n-1}}^{t_n} \int_{\Omega} \mathbf{S}^n \nabla c_h^n(\mathbf{x}) \nabla \psi(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t$  and introduce

$$T_{D_2} := \sum_{n=1}^{N} \int_{t_{n-1}}^{t_n} \sum_{K \in \mathscr{T}_h} \int_{K} \mathbf{S}^n \nabla c_h^n(\mathbf{x}) \cdot \left( \nabla \psi(\mathbf{x}, t_{n-1}) - \nabla \psi(\mathbf{x}, t) \right) d\mathbf{x} dt$$
  
$$T_{D_3} := \int_0^T \sum_{K \in \mathscr{T}_h} \int_{K} \mathbf{S}_{\triangle t} \nabla c_{h, \triangle t}(\mathbf{x}, t) \cdot \nabla \psi(\mathbf{x}, t) d\mathbf{x} dt$$
  
$$- \int_0^T \int_{\Omega} \mathbf{S} \nabla c(\mathbf{x}, t) \cdot \nabla \psi(\mathbf{x}, t) d\mathbf{x} dt ,$$

where  $c_{h,\Delta t}$  is given by (5.4). Clearly, (6.11) is valid when  $T_{D_2}$  and  $T_{D_3}$  tend to zero as  $h, \Delta t \to 0$ . We first estimate  $T_{D_2}$ . We have, for  $t \in (t_{n-1}, t_n]$ ,

$$\nabla \psi(\mathbf{x}, t_{n-1}) - \nabla \psi(\mathbf{x}, t) | \leq g(\Delta t)$$

where g satisfies  $g(\triangle t) > 0$  and  $g(\triangle t) \rightarrow 0$  as  $\triangle t \rightarrow 0$ . Thus

$$|T_{D_2}| \leq C_{\mathbf{S}}g(\triangle t) \sum_{n=1}^N \triangle t_n \sum_{K \in \mathscr{T}_h} \left| \nabla c_h^n |_K \right| |K| \leq C_{\mathbf{S}}g(\triangle t) \left(\frac{C_{\mathrm{ae}}}{c_{\mathbf{S}}}\right)^{\frac{1}{2}} T^{\frac{1}{2}} |\Omega|^{\frac{1}{2}},$$

using the Cauchy–Schwarz inequality and the a priori estimate (5.3).

To show that  $T_{D_3} \rightarrow 0$  as  $h, \triangle t \rightarrow 0$ , we begin by showing that

$$T'_{D_3} := \int_0^T \sum_{K \in \mathscr{T}_h} \int_K \left( \nabla c_{h, \bigtriangleup t}(\mathbf{x}, t) - \nabla c(\mathbf{x}, t) \right) \cdot \mathbf{w}(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \longrightarrow 0 \tag{6.12}$$

as  $h, \triangle t \to 0$  for all  $\mathbf{w} \in [C^1(\overline{Q_T})]^d$ . To this purpose, we first rewrite  $T'_{D_3}$  as

$$T'_{D_3} = \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \sum_{K \in \mathscr{T}_h} \int_K \nabla c_h^n(\mathbf{x}) \cdot \mathbf{w}(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t + \int_0^T \int_\Omega c(\mathbf{x},t) \nabla \cdot \mathbf{w}(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \,,$$

where we have used the Green theorem for c (recall that  $c \in L^2(0,T;H^1_0(\Omega))$  by Theorem 6.1) and w. We easily notice that we cannot use the Green theorem for  $c_h^n$  on  $\Omega$ , since  $c_h^n \notin H^1(\Omega)$ . We are thus forced to apply it on each  $K \in \mathcal{T}_h$ .

We rewrite the first term of  $T'_{D_3}$  as

$$\sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} \sum_{K \in \mathscr{T}_{h}} \int_{K} -c_{h}^{n}(\mathbf{x}) \nabla \cdot \mathbf{w}(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t + \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} \sum_{K \in \mathscr{T}_{h}} \int_{\partial K} c_{h}^{n}(\mathbf{x}) \mathbf{w}(\mathbf{x},t) \cdot \mathbf{n} \, \mathrm{d}\gamma(\mathbf{x}) \, \mathrm{d}t$$

We next consider the term

$$T_{D_3}'' := \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \sum_{K \in \mathscr{T}_h} \int_{\partial K} c_h^n \mathbf{w} \cdot \mathbf{n} \, \mathrm{d}\gamma(\mathbf{x}) \, \mathrm{d}t \,.$$
(6.13)

Reordering the summation by sides, we come to

$$T_{D_3}'' = \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \Big( \sum_{\sigma_{K,L} \in \mathscr{E}_h^{\text{int}}} \int_{\sigma_{K,L}} (c_h^n |_K - c_h^n |_L) \mathbf{w} \cdot \mathbf{n}_{K,L} \, \mathrm{d} \boldsymbol{\gamma}(\mathbf{x}) \\ + \sum_{\sigma_K \in \mathscr{E}_h^{\text{ext}}} \int_{\sigma_K} c_h^n |_K \mathbf{w} \cdot \mathbf{n}_K \, \mathrm{d} \boldsymbol{\gamma}(\mathbf{x}) \Big) \, \mathrm{d}t \,,$$

where we have used  $\mathbf{w} \cdot \mathbf{n}_{K,L} = -\mathbf{w} \cdot \mathbf{n}_{L,K}$  following from  $\mathbf{w} \in [C^1(\overline{Q_T})]^d$ . The functions  $c_h^n|_K - c_h^n|_L$  or  $c_h^n|_K$  restricted to a side  $\sigma_{K,L} \in \mathscr{E}_h^{\text{int}}$  or  $\sigma_K \in \mathscr{E}_h^{\text{ext}}$ , respectively, are first-order polynomials, vanishing in the barycentre  $Q_D$  of this side. For  $\sigma_{K,L} \in \mathscr{E}_h^{\text{int}}$ , this follows from the continuity requirement given in the definition of  $X_h$  and for  $\sigma_K \in \mathscr{E}_h^{\text{ext}}$  from the zero Dirichlet boundary condition imposed by (3.6b). Hence

$$\int_{\sigma_{K,L}} \left( c_h^n |_K(\mathbf{x}) - c_h^n|_L(\mathbf{x}) \right) \mathrm{d}\gamma(\mathbf{x}) = 0, \quad \int_{\sigma_K} c_h^n |_K(\mathbf{x}) \,\mathrm{d}\gamma(\mathbf{x}) = 0 \tag{6.14}$$

for all  $\sigma_{K,L} \in \mathscr{E}_h^{\text{int}}$  and  $\sigma_K \in \mathscr{E}_h^{\text{ext}}$ , since the quadrature formula using the value in the barycentre of a segment (d = 2) or a triangle (d = 3) is precise for linear functions. We further estimate

$$\left|c_{h}^{n}|_{K}(\mathbf{x})\right| = \left|c_{h}^{n}|_{K}(\mathbf{x}) - c_{h}^{n}|_{K}(Q_{D})\right| \le \left|\nabla c_{h}^{n}|_{K}\right| |\mathbf{x} - Q_{D}| \le \left|\nabla c_{h}^{n}|_{K}\right| \frac{\operatorname{diam}(\boldsymbol{\sigma}_{K})}{4 - d},$$

with  $\mathbf{x} \in \sigma_K \in \mathscr{E}_h^{\text{ext}}$ , where we have used  $|\mathbf{x} - Q_D| \leq \text{diam}(\sigma_K)/2$  for d = 2 but only  $|\mathbf{x} - Q_D| \leq \text{diam}(\sigma_K)$  for d = 3. Similarly,

$$\left|c_{h}^{n}|_{K}(\mathbf{x})-c_{h}^{n}|_{L}(\mathbf{x})\right| \leq \left|\nabla c_{h}^{n}|_{K}\right|\frac{\operatorname{diam}(\sigma_{K,L})}{4-d}+\left|\nabla c_{h}^{n}|_{L}\right|\frac{\operatorname{diam}(\sigma_{K,L})}{4-d}$$

with  $\mathbf{x} \in \sigma_{K,L} \in \mathscr{E}_h^{\text{int}}$ . We have from the smoothness of  $\mathbf{w}$ 

$$\mathbf{w} \cdot \mathbf{n}_{\sigma_D}(\mathbf{x}) = \mathbf{w} \cdot \mathbf{n}_{\sigma_D}(Q_D) + f(\xi) |Q_D - \mathbf{x}| \qquad \mathbf{x} \in \sigma_D \in \mathscr{E}_h, \, \xi \in [Q_D, \mathbf{x}]$$

with  $|f(\xi)| \leq C_{\mathbf{w}}$ . Thus

$$\int_{\sigma_K} c_h^n |_K(\mathbf{x}) f(\boldsymbol{\xi})| Q_D - \mathbf{x} | \, \mathrm{d} \boldsymbol{\gamma}(\mathbf{x}) \le C_{\mathbf{w}} \left( \frac{\operatorname{diam}(\sigma_K)}{4 - d} \right)^2 \left| \nabla c_h^n |_K \right| |\sigma_K|$$

for an exterior side  $\sigma_K$  and similarly

$$\begin{split} \int_{\boldsymbol{\sigma}_{K,L}} & \left( c_h^n |_K(\mathbf{x}) - c_h^n |_L(\mathbf{x}) \right) f(\boldsymbol{\xi}) | \mathcal{Q}_D - \mathbf{x} | \, \mathrm{d}\boldsymbol{\gamma}(\mathbf{x}) \leq C_{\mathbf{w}} \Big( \frac{\operatorname{diam}(\boldsymbol{\sigma}_{K,L})}{4 - d} \Big)^2 \\ & \left( \left| \nabla c_h^n |_K \right| + \left| \nabla c_h^n |_L \right| \right) | \boldsymbol{\sigma}_{K,L} \end{split}$$

for an interior side  $\sigma_{K,L}$ . Using these estimates, we immediately come to

$$\begin{split} |T_{D_3}''| &\leq C_{\mathbf{w}} \frac{h}{(4-d)^2} \frac{d+1}{d-1} \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \sum_{K \in \mathscr{T}_h} \left| \nabla c_h^n |_K \right| \operatorname{diam}(K)^d \, \mathrm{d}t \\ &\leq \frac{C_{\mathbf{w}}}{\kappa_{\mathscr{T}}} \frac{h}{(4-d)^2} \frac{d+1}{d-1} \sum_{n=1}^N \triangle t_n \sum_{K \in \mathscr{T}_h} \left| \nabla c_h^n |_K \right| |K| \\ &\leq \frac{C_{\mathbf{w}}}{\kappa_{\mathscr{T}}} \frac{h}{(4-d)^2} \frac{d+1}{d-1} \left( \frac{C_{\mathrm{ae}}}{c_{\mathbf{S}}} \right)^{\frac{1}{2}} T^{\frac{1}{2}} |\Omega|^{\frac{1}{2}}, \end{split}$$

using the fact that each  $\nabla c_h^n|_K$  is in the summation over all sides just (d+1)times,  $|\sigma_D| \leq \operatorname{diam}(K)^{d-1}/(d-1)$  and  $\operatorname{diam}(\sigma_D) \leq \operatorname{diam}(K) \leq h$  for all  $\sigma_D \in \mathscr{E}_K$ , Assumption (B), the Cauchy–Schwarz inequality, and the a priori estimate (5.3). Thus  $T_{D_3}'' \to 0$  as  $h \to 0$ .

To conclude that  $T'_{D_3} \to 0$  as  $h, \triangle t \to 0$ , it remains to show that

$$-\sum_{n=1}^{N}\int_{t_{n-1}}^{t_{n}}\sum_{K\in\mathscr{T}_{h}}\int_{K}c_{h}^{n}(\mathbf{x})\nabla\cdot\mathbf{w}(\mathbf{x},t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t+\int_{0}^{T}\int_{\Omega}c(\mathbf{x},t)\nabla\cdot\mathbf{w}(\mathbf{x},t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t\longrightarrow0.$$

This is however immediate, since we can rewrite it as

$$\int_0^T \int_\Omega (c(\mathbf{x},t) - c_{h,\triangle t}(\mathbf{x},t)) \nabla \cdot \mathbf{w}(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \longrightarrow 0$$

which is a consequence of the strong  $L^2(Q_T)$  convergence of  $c_{h, \Delta t}$  to c.

We next show that the density of the set  $[C^1(\overline{Q_T})]^d$  in  $[L^2(Q_T)]^d$  and (6.12) implies a weak convergence of  $\nabla c_{h, \triangle t}$  (piecewise constant function in space and time) to  $\nabla c$ . Indeed, let  $\mathbf{w} \in [L^2(Q_T)]^d$  be given and let  $\mathbf{w}_n$  be a sequence of  $[C^1(\overline{Q_T})]^d$  functions converging in  $[L^2(Q_T)]^d$  to w. Then

$$\int_0^T \int_{\Omega} (\nabla c_{h, \Delta t} - \nabla c) \cdot \mathbf{w} \, \mathrm{d}\mathbf{x} \, \mathrm{d}t = \int_0^T \int_{\Omega} (\nabla c_{h, \Delta t} - \nabla c) \cdot \mathbf{w}_n \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \\ + \int_0^T \int_{\Omega} (\nabla c_{h, \Delta t} - \nabla c) \cdot (\mathbf{w} - \mathbf{w}_n) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t.$$

The second term of the above expression tends to zero as  $n \rightarrow \infty$  by the Cauchy– Schwarz inequality. Hence the whole expression tends to zero as  $h, \triangle t \rightarrow 0$  for each  $\mathbf{w} \in [L^2(Q_T)]^d$ , using (6.12) for the first term. We now finally conclude that  $T_{D_3} \to 0$  as  $h, \triangle t \to 0$ . We can write

$$T_{D_3} = \int_0^T \int_{\Omega} (\mathbf{S}_{\triangle t} - \mathbf{S}) \nabla c_{h, \triangle t} \cdot \nabla \psi \, \mathrm{d} \mathbf{x} \, \mathrm{d} t - \int_0^T \int_{\Omega} \mathbf{S} (\nabla c - \nabla c_{h, \triangle t}) \cdot \nabla \psi \, \mathrm{d} \mathbf{x} \, \mathrm{d} t \, .$$

Since  $(\mathbf{S}_{\Delta t})_{i,j}$ ,  $1 \le i, j \le d$ , converge strongly in  $L^1(Q_T)$  to  $\mathbf{S}_{i,j}$  by its definition (6.9), the boundedness of  $\mathbf{S}_{\Delta t}$  and  $\mathbf{S}$  given by Assumption (A3) implies a strong  $L^2(Q_T)$  convergence as well. Hence the first term of the above expression tends to zero as  $h, \Delta t \to 0$ , using the boundedness of  $|\nabla \psi|$ , the a priori estimate (5.3), and the Cauchy–Schwarz inequality. The second term converges to

zero by the  $L^{\infty}$  boundedness of **S** and the weak convergence of  $\nabla c_{h, \Delta t}$  to  $\nabla c$  shown in the previous paragraph. Altogether, combining (6.10) and (6.11) gives

$$T_D \longrightarrow \int_0^T \int_{\Omega} \mathbf{S} \nabla c(\mathbf{x}, t) \cdot \nabla \psi(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \text{ as } h, \Delta t \to 0.$$
 (6.15)

*Remark 6.2 (Nonconforming approximation)* The fact that  $T''_{D_3}$  given by (6.13) is not immediately equal to zero is the consequence of the nonconforming-type approximation. However, since the approximation is continuous in the barycentres of interior sides and equal to zero in the barycentres of exterior sides, (6.14) is fulfilled and consequently  $T''_{D_3}$  is of order *h*, which suffices for the convergence.

## Convection term

We recall that

$$T_C = \sum_{n=1}^N \triangle t_n \sum_{D \in \mathscr{D}_h} \sum_{E \in \mathscr{N}(D)} v_{D,E}^n \overline{c_{D,E}^n} \, \Psi(Q_D, t_{n-1})$$

and denote

$$\mathbf{v}^{n}(\mathbf{x}) := \frac{1}{\bigtriangleup t_{n}} \int_{t_{n-1}}^{t_{n}} \mathbf{v}(\mathbf{x}, t) \, \mathrm{d}t \qquad n \in \{1, 2, \dots, N\}, \, \mathbf{x} \in \Omega.$$
(6.16)

We first intend to show that

$$T_{C} + \sum_{n=1}^{N} \triangle t_{n} \sum_{D \in \mathscr{D}_{h}} c_{D}^{n} \sum_{E \in \mathscr{N}(D)} \int_{\sigma_{D,E}} \mathbf{v}^{n}(\mathbf{x}) \cdot \mathbf{n}_{D,E} \, \psi(\mathbf{x}, t_{n-1}) \, \mathrm{d}\gamma(\mathbf{x}) \quad (6.17)$$
$$- \sum_{n=1}^{N} \triangle t_{n} \sum_{D \in \mathscr{D}_{h}} c_{D}^{n} \int_{D} \nabla \cdot \mathbf{v}^{n}(\mathbf{x}) \, \psi(\mathbf{x}, t_{n-1}) \, \mathrm{d}\mathbf{x} \longrightarrow 0 \text{ as } h \to 0.$$

We add and subtract  $c_D^n \psi(Q_D, t_{n-1}) v_{D,E}^n$  and  $\overline{c_{D,E}^n} \int_{\sigma_{D,E}} \mathbf{v}^n(\mathbf{x}) \cdot \mathbf{n}_{D,E} \psi(\mathbf{x}, t_{n-1}) \, d\gamma(\mathbf{x})$  to the summations in the first two terms of (6.17). We denote

$$\begin{split} T_{C_1} &:= \sum_{n=1}^N \bigtriangleup t_n \sum_{D \in \mathscr{D}_h} \sum_{E \in \mathscr{N}(D)} (\overline{c_{D,E}^n} - c_D^n) \Big( \Psi(\mathcal{Q}_D, t_{n-1}) v_{D,E}^n \\ &- \int_{\sigma_{D,E}} \mathbf{v}^n(\mathbf{x}) \cdot \mathbf{n}_{D,E} \, \Psi(\mathbf{x}, t_{n-1}) \, \mathrm{d} \boldsymbol{\gamma}(\mathbf{x}) \Big) \,, \\ T_{C_2} &:= \sum_{n=1}^N \bigtriangleup t_n \sum_{D \in \mathscr{D}_h} \sum_{E \in \mathscr{N}(D)} \overline{c_{D,E}^n} \int_{\sigma_{D,E}} \mathbf{v}^n(\mathbf{x}) \cdot \mathbf{n}_{D,E} \, \Psi(\mathbf{x}, t_{n-1}) \, \mathrm{d} \boldsymbol{\gamma}(\mathbf{x}) \,, \\ T_{C_3} &:= \sum_{n=1}^N \bigtriangleup t_n \sum_{D \in \mathscr{D}_h} c_D^n \Psi(\mathcal{Q}_D, t_{n-1}) \sum_{E \in \mathscr{N}(D)} v_{D,E}^n \,, \\ T_{C_4} &:= \sum_{n=1}^N \bigtriangleup t_n \sum_{D \in \mathscr{D}_h} c_D^n \int_D \nabla \cdot \mathbf{v}^n(\mathbf{x}) \, \Psi(\mathbf{x}, t_{n-1}) \, \mathrm{d} \mathbf{x} \,. \end{split}$$

One can easily verify that (6.17) is satisfied when  $T_{C_1} \rightarrow 0$ ,  $T_{C_2} \rightarrow 0$ , and  $(T_{C_3} T_{C_4}$ )  $\rightarrow 0$  as  $h \rightarrow 0$ . We begin with  $T_{C_2}$ . We denote

$$\mathbf{v}_{\psi;D,E}^n := \int_{\sigma_{D,E}} \mathbf{v}^n(\mathbf{x}) \cdot \mathbf{n}_{D,E} \, \psi(\mathbf{x},t_{n-1}) \, \mathrm{d}\gamma(\mathbf{x}) \, .$$

Since the summation in  $T_{C_2}$  is over all  $D \in \mathcal{D}_h$  and all its neighbors, each interior dual side is in the summation just twice. We consider one fixed interior dual side  $\sigma_{D,E}$ , where we have denoted D and E such that  $v_{D,E}^n \ge 0$ , and have

$$\left(c_D^n + \alpha_{D,E}^n(c_E^n - c_D^n)\right)\mathbf{v}_{\psi;D,E}^n + \left(c_D^n + \alpha_{D,E}^n(c_E^n - c_D^n)\right)\mathbf{v}_{\psi;E,D}^n = 0$$

considering the definition of the local Péclet upstream weighting (3.7) and the fact that  $\mathbf{v}_{\psi;D,E}^n = -\mathbf{v}_{\psi;E,D}^n$ . Thus  $T_{C_2} = 0$ . Next we consider  $T_{C_3}$  and  $T_{C_4}$ . We immediately have that

$$\sum_{E \in \mathscr{N}(D)} v_{D,E}^n = \int_D \nabla \cdot \mathbf{v}^n(\mathbf{x}) \, \mathrm{d} \mathbf{x} \qquad \forall D \in \mathscr{D}_h^{int} \,,$$

using the definition of  $v_{D,E}^n$ . We further estimate

$$\begin{aligned} |T_{C_3} - T_{C_4}| &= \left| \sum_{n=1}^N \bigtriangleup t_n \sum_{D \in \mathscr{D}_h^{int}} c_D^n \int_D \nabla \cdot \mathbf{v}^n(\mathbf{x}) \left( \psi(\mathcal{Q}_D, t_{n-1}) - \psi(\mathbf{x}, t_{n-1}) \right) d\mathbf{x} \right| \\ &\leq C_{2,\psi} h \sum_{n=1}^N \sum_{D \in \mathscr{D}_h} |c_D^n| \int_{t_{n-1}}^{t_n} \int_D r(\mathbf{x}, t) d\mathbf{x} dt \qquad (6.18) \\ &\leq C_{2,\psi} h \left( \sum_{n=1}^N \sum_{D \in \mathscr{D}_h} \bigtriangleup t_n |D| (c_D^n)^2 \right)^{\frac{1}{2}} \left( \sum_{n=1}^N \sum_{D \in \mathscr{D}_h} \frac{\left( \int_{t_{n-1}}^{t_n} \int_D r(\mathbf{x}, t) d\mathbf{x} dt \right)^2}{\bigtriangleup t_n |D|} \right)^{\frac{1}{2}} \\ &\leq C_{2,\psi} h \left( \frac{C_{ae}}{c_\beta} T \right)^{\frac{1}{2}} \|r\|_{0,\mathcal{Q}_T}, \end{aligned}$$

considering the boundary condition  $c_D^n = 0$  for all  $D \in \mathscr{D}_h^{ext}$ ,

$$\psi(Q_D, t_{n-1}) - \psi(\mathbf{x}, t_{n-1}) | \le C_{2,\psi} h \tag{6.19}$$

for all  $\mathbf{x} \in D$ ,

$$\int_{D} |\nabla \cdot \mathbf{v}^{n}(\mathbf{x})| \, \mathrm{d}\mathbf{x} = \frac{1}{\triangle t_{n}} \int_{D} \int_{t_{n-1}}^{t_{n}} \nabla \cdot \mathbf{v}(\mathbf{x},t) \, \mathrm{d}t \, \mathrm{d}\mathbf{x} = \frac{1}{\triangle t_{n}} \int_{D} \int_{t_{n-1}}^{t_{n}} r(\mathbf{x},t) \, \mathrm{d}t \, \mathrm{d}\mathbf{x},$$

which follows from Assumption (A4), the Cauchy-Schwarz inequality, and the a priori estimate (5.1). Thus  $(T_{C_3} - T_{C_4}) \rightarrow 0$  as  $h \rightarrow 0$ . We finally turn to  $T_{C_1}$ . We first define

$$T_{C_5} := \sum_{n=1}^N \triangle t_n \sum_{D \in \mathscr{D}_h} \sum_{E \in \mathscr{N}(D)} \operatorname{diam}(K_{D,E})^{d-2} (\overline{c_{D,E}^n} - c_D^n)^2.$$

We have

$$(\overline{c_{D,E}^{n}} - c_{D}^{n})^{2} = \left(\alpha_{D,E}^{n}(c_{E}^{n} - c_{D}^{n})\right)^{2} \le \frac{1}{4}(c_{E}^{n} - c_{D}^{n})^{2}$$

when  $v_{D,E}^n \ge 0$ , considering the definition of the local Péclet upstream weighting (3.7) and Remark 3.1, which gives  $0 \le \alpha_{D,E}^n \le 1/2$ . Similarly, when  $v_{D,E}^n < 0$ , we come to

$$(\overline{c_{D,E}^n} - c_D^n)^2 = \left( (c_E^n - c_D^n)(1 - \alpha_{D,E}^n) \right)^2 \le (c_E^n - c_D^n)^2.$$

We have

$$T_{C_5} \leq 2\sum_{n=1}^{N} \triangle t_n \sum_{\sigma_{D,E} \in \mathscr{F}_h^{\text{int}}} \operatorname{diam}(K_{D,E})^{d-2} (c_E^n - c_D^n)^2$$
$$\leq \frac{d+1}{d\kappa_{\mathscr{T}}} \sum_{n=1}^{N} \triangle t_n \|c_h^n\|_{X_h}^2 \leq \frac{d+1}{d\kappa_{\mathscr{T}}} \frac{C_{\text{ae}}}{c_{\mathbf{S}}},$$

noticing that each interior dual side is in the original summation just twice and using the estimate (3.3) and the a priori estimate (5.3). We next define

$$T_{C_6} := \sum_{n=1}^{N} \triangle t_n \sum_{D \in \mathscr{D}_h} \sum_{E \in \mathscr{N}(D)} \frac{1}{\operatorname{diam}(K_{D,E})^{d-2}} \left( \int_{\sigma_{D,E}} \mathbf{v}^n(\mathbf{x}) \cdot \mathbf{n}_{D,E} \Big( \psi(Q_D, t_{n-1}) - \psi(\mathbf{x}, t_{n-1}) \Big) \, \mathrm{d}\gamma(\mathbf{x}) \Big)^2$$

and estimate

$$T_{C_{6}} \leq C_{2,\psi}^{2}h^{2}C_{\mathbf{v}}^{2}\sum_{n=1}^{N} \triangle t_{n}\sum_{D \in \mathscr{D}_{h}} \sum_{E \in \mathscr{N}(D)} \frac{1}{\operatorname{diam}(K_{D,E})^{d-2}} |\sigma_{D,E}|^{2}$$
  
$$\leq C_{2,\psi}^{2}h^{2}C_{\mathbf{v}}^{2}\frac{(d+1)d}{(d-1)^{2}}\sum_{n=1}^{N} \triangle t_{n}\sum_{K \in \mathscr{T}_{h}} \operatorname{diam}(K)^{d} \leq C_{2,\psi}^{2}h^{2}\frac{C_{\mathbf{v}}^{2}}{\kappa_{\mathscr{T}}}\frac{(d+1)d}{(d-1)^{2}} |\Omega|T,$$

using (6.19),  $|v_{D,E}^n| \leq C_v |\sigma_{D,E}|$  following from Assumption (A4), (3.5), noticing that each interior dual side is in the original summation just twice and that each  $K \in \mathcal{T}_h$  contains exactly (d+1)d/2 dual sides, and finally Assumption (B). We now notice that

$$T_{C_1}^2 \le T_{C_5} T_{C_6}$$

using the Cauchy–Schwarz inequality, and hence  $T_{C_1} \rightarrow 0$  as  $h \rightarrow 0$ . Thus (6.17) is satisfied.

Using the Green theorem and considering  $c_D^n = 0$  for all  $D \in \mathscr{D}_h^{ext}$ , we easily come to

$$\sum_{n=1}^{N} \triangle t_n \sum_{D \in \mathscr{D}_h} c_D^n \sum_{E \in \mathscr{N}(D)} \int_{\sigma_{D,E}} \mathbf{v}^n(\mathbf{x}) \cdot \mathbf{n}_{D,E} \, \boldsymbol{\psi}(\mathbf{x}, t_{n-1}) \, \mathrm{d}\boldsymbol{\gamma}(\mathbf{x}) = \sum_{n=1}^{N} \triangle t_n \qquad (6.20)$$

$$\sum_{D\in\mathscr{D}_h} c_D^n \int_D \mathbf{v}^n(\mathbf{x}) \nabla \psi(\mathbf{x}, t_{n-1}) \, \mathrm{d}\mathbf{x} + \sum_{n=1}^N \triangle t_n \sum_{D\in\mathscr{D}_h} c_D^n \int_D \nabla \cdot \mathbf{v}^n(\mathbf{x}) \psi(\mathbf{x}, t_{n-1}) \, \mathrm{d}\mathbf{x}$$

Therefore it follows from (6.17) that if we can prove that

$$\sum_{n=1}^{N} \triangle t_n \sum_{D \in \mathscr{D}_h} c_D^n \int_D \mathbf{v}^n(\mathbf{x}) \cdot \nabla \boldsymbol{\psi}(\mathbf{x}, t_{n-1}) \, \mathrm{d}\mathbf{x}$$

$$\rightarrow \int_0^T \int_\Omega c(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t) \cdot \nabla \boldsymbol{\psi}(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \text{ as } h, \triangle t \to 0,$$
(6.21)

then we will have that

$$T_C \longrightarrow -\int_0^T \int_{\Omega} c(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t) \cdot \nabla \psi(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \text{ as } h, \Delta t \to 0.$$
 (6.22)

To prove (6.21), we introduce

$$T_{C_7} := \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \int_{\Omega} \tilde{c}_{h, \Delta t}(\mathbf{x}, t) \mathbf{v}^n(\mathbf{x}) \cdot \left(\nabla \psi(\mathbf{x}, t_{n-1}) - \nabla \psi(\mathbf{x}, t)\right) d\mathbf{x} dt ,$$
  

$$T_{C_8} := \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \int_{\Omega} \left(\tilde{c}_{h, \Delta t}(\mathbf{x}, t) - c(\mathbf{x}, t)\right) \mathbf{v}^n(\mathbf{x}) \cdot \nabla \psi(\mathbf{x}, t) d\mathbf{x} dt ,$$
  

$$T_{C_9} := \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \int_{\Omega} c(\mathbf{x}, t) \left(\mathbf{v}^n(\mathbf{x}) - \mathbf{v}(\mathbf{x}, t)\right) \cdot \nabla \psi(\mathbf{x}, t) d\mathbf{x} dt .$$

We have

$$|\nabla \psi(\mathbf{x}, t_{n-1}) - \nabla \psi(\mathbf{x}, t)| \le g(\triangle t)$$

for  $t \in (t_{n-1}, t_n]$  and thus

$$|T_{C_7}| \leq g(\triangle t) \sum_{n=1}^N \sum_{D \in \mathscr{D}_h} |c_D^n| \int_D \int_{t_{n-1}}^{t_n} |\mathbf{v}(\mathbf{x},t)| \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \leq g(\triangle t) \left(\frac{C_{\mathrm{ae}}}{c_\beta}T\right)^{\frac{1}{2}} \|\mathbf{v}\|_{0,Q_T},$$

using the same estimate as in (6.18). Thus  $T_{C_7} \to 0$  as  $\triangle t \to 0$ . It is immediate that  $T_{C_8} \to 0$  as  $h, \triangle t \to 0$ , using the strong (and consequently weak) convergence of  $\tilde{c}_{h,\triangle t}$  to c. By Assumption (A4) and (6.16) **v** and **v**<sup>n</sup> are bounded, and hence the piecewise constant in time approximation given by **v**<sup>n</sup> converges strongly in  $\mathbf{L}^2(Q_T)$  to **v** as  $\triangle t \to 0$ . Since  $|\nabla \psi| \leq C_{2,\psi}$  and  $c \in L^2(Q_T)$ , it suffices to use the Cauchy–Schwarz inequality to conclude that  $T_{C_9} \to 0$  as  $\triangle t \to 0$ . Thus (6.21) and consequently (6.22) is fulfilled.

## Reaction term

We would now like to show that

$$T_R \longrightarrow \int_0^T \int_{\Omega} F(c(\mathbf{x},t)) \psi(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \text{ as } h, \Delta t \to 0.$$
 (6.23)

For this purpose, we introduce

$$T_{R_1} := \sum_{n=1}^N \sum_{D \in \mathscr{D}_h} F(c_D^n) \int_{t_{n-1}}^{t_n} \int_D \left( \psi(Q_D, t_{n-1}) - \psi(\mathbf{x}, t) \right) d\mathbf{x} dt ,$$
  
$$T_{R_2} := \sum_{n=1}^N \sum_{D \in \mathscr{D}_h} \int_{t_{n-1}}^{t_n} \int_D \left( F(c_D^n) - F(c(\mathbf{x}, t)) \right) \psi(\mathbf{x}, t) d\mathbf{x} dt .$$

We have

$$|\psi(Q_D, t_{n-1}) - \psi(\mathbf{x}, t)| \le C_{3, \psi}(h + \Delta t)$$
(6.24)

for all  $\mathbf{x} \in D$  and  $t \in (t_{n-1}, t_n]$ , and thus

$$|T_{R_1}| \leq C_{3,\psi} L_F(h + \Delta t) \sum_{n=1}^N \sum_{D \in \mathscr{D}_h} \Delta t_n |D| |c_D^n| \leq C_{3,\psi} L_F(h + \Delta t) \left(\frac{C_{ae}}{c_\beta} T\right)^{\frac{1}{2}} |\Omega|^{\frac{1}{2}} T^{\frac{1}{2}},$$

using the Lipschitz continuity of *F*, following from Assumption (A5) or (A6), the Cauchy–Schwarz inequality, and the a priori estimate (5.1). Hence,  $T_{R_1} \rightarrow 0$  as  $h, \triangle t \rightarrow 0$ . We have

$$|T_{R_2}| \leq C_{1,\psi} L_F \int_0^T \int_{\Omega} |\tilde{c}_{h,\triangle t}(\mathbf{x},t) - c(\mathbf{x},t)| \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \,,$$

which tends to 0 because of the strong  $L^2(Q_T)$  convergence of  $\tilde{c}_{h, \Delta t}$  to *c*. Thus, (6.23) is fulfilled.

## Sources term

We finally show that

$$T_{S} \longrightarrow \int_{0}^{T} \int_{\Omega} q(\mathbf{x}, t) \psi(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \text{ as } h, \Delta t \to 0.$$
 (6.25)

We set

$$T_{S_1} := \sum_{n=1}^{N} \sum_{D \in \mathscr{D}_h} q_D^n \int_{t_{n-1}}^{t_n} \int_D \left( \psi(Q_D, t_{n-1}) - \psi(\mathbf{x}, t) \right) d\mathbf{x} dt ,$$
  
$$T_{S_2} := \sum_{n=1}^{N} \sum_{D \in \mathscr{D}_h} \int_{t_{n-1}}^{t_n} \int_D \left( q_D^n - q(\mathbf{x}, t) \right) \psi(\mathbf{x}, t) d\mathbf{x} dt .$$

We can bound  $|T_{S_1}|$  by

$$C_{3,\psi}(h+\triangle t)\sum_{n=1}^{N}\sum_{D\in\mathscr{D}_{h}}\int_{t_{n-1}}^{t_{n}}\int_{D}|q(\mathbf{x},t)|\,\mathrm{d}\mathbf{x}\,\mathrm{d}t\leq C_{3,\psi}(h+\triangle t)\|q\|_{0,\mathcal{Q}_{T}}|\Omega|^{\frac{1}{2}}T^{\frac{1}{2}},$$

using (6.24) and the Cauchy–Schwarz inequality. Finally,

$$|T_{S_2}| \leq C_{1,\psi} \sum_{n=1}^N \sum_{D \in \mathscr{D}_h} \int_{t_{n-1}}^{t_n} \int_D |q_D^n - q(\mathbf{x},t)| \, \mathrm{d}\mathbf{x} \, \mathrm{d}t \, ,$$

which tends to 0 as  $h, \triangle t \rightarrow 0$  because of the  $L^1$  convergence of the piecewise constant approximation  $q_D^n$  to q. Thus (6.25) is satisfied.

We are now ready to give the final theorem of this paper:

**Theorem 6.2 (Convergence to a weak solution)** There exist subsequences of  $\tilde{c}_{h,\Delta t}$  and  $c_{h,\Delta t}$ , the approximate solutions of the problem (1.1)–(2.2) by means of the combined finite volume–nonconforming/mixed-hybrid finite element scheme given by Definition 5.1, which converge strongly in  $L^2(Q_T)$  to a weak solution of the problem (1.1)–(2.2) given by Definition 2.1. If the weak solution is unique, then the whole sequences  $\tilde{c}_{h,\Delta t}$ ,  $c_{h,\Delta t}$  converge to the weak solution.

*Proof* We have from Theorem 6.1 that subsequences of  $\tilde{c}_{h,\Delta t}$  and  $c_{h,\Delta t}$  converge strongly in  $L^2(Q_T)$  to some function  $c \in L^2(0,T;H_0^1(\Omega))$ . The function c satisfies

$$-\int_{0}^{T} \int_{\Omega} \beta(c(\mathbf{x},t)) \psi_{t}(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t - \int_{\Omega} \beta(c_{0}(\mathbf{x})) \psi(\mathbf{x},0) \, \mathrm{d}\mathbf{x}$$
$$+ \int_{0}^{T} \int_{\Omega} \mathbf{S}(\mathbf{x},t) \nabla c(\mathbf{x},t) \cdot \nabla \psi(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t - \int_{0}^{T} \int_{\Omega} c(\mathbf{x},t) \mathbf{v}(\mathbf{x},t) \cdot \nabla \psi(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t$$
$$+ \int_{0}^{T} \int_{\Omega} F(c(\mathbf{x},t)) \psi(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t = \int_{0}^{T} \int_{\Omega} q(\mathbf{x},t) \psi(\mathbf{x},t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t$$

for all test functions  $\psi \in \Psi$ , given by (6.1). This follows from (6.8), (6.15), (6.22), (6.23), (6.25), and (6.2). In addition,  $\beta(c) \in L^{\infty}(0,T;L^{2}(\Omega))$ , which follows from (5.2). Thus *c* is a weak solution of the problem (1.1)–(2.2), since  $\Psi$  is dense in the set { $\varphi$ ;  $\varphi \in L^{2}(0,T;H_{0}^{1}(\Omega))$ ,  $\varphi_{t} \in L^{\infty}(Q_{T})$ ,  $\varphi(\cdot,T) = 0$ }.  $\Box$ 

## 7 Numerical experiments

We present the results of two numerical experiments in this section. We first check our scheme for a model problem with a traveling wave solution and then consider a problem with an inhomogeneous and anisotropic diffusion–dispersion tensor and compare our scheme with three different ones. The computations were done in double precision on a notebook with Intel Pentium 4-M 1.8 GHz processor and MS Windows XP operating system. Machine precision was in power of  $10^{-16}$ .

## 7.1 A model problem with a traveling wave solution

We consider here a model degenerate parabolic convection-diffusion problem with a known traveling wave solution (cf. [34]). In particular, we take the equation (1.1) for  $\Omega = (0, 1) \times (0, 1)$  and T = 1 with

$$\beta(c) = c^{\frac{1}{2}} \text{ for } c \ge 0,$$
  

$$\mathbf{S} = \delta \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$
  

$$\mathbf{v} = (v, 0),$$
  

$$F(c) = 0, q = 0.$$

Here,  $\delta > 0$  and  $\nu > 0$  are parameters. We fix  $\nu$  to 0.8 and let  $\delta$  vary: for large values of  $\delta$ , diffusion dominates over convection and conversely for small values



Fig. 7.1 Initial space mesh  $\mathcal{T}_h$  (solid) and its dual mesh  $\mathcal{D}_h$  (dashed) with emplacement of the unknowns

of  $\delta$ . The initial and Dirichlet boundary conditions are given by the exact solution

$$c(x,y,t) = \left(1 - e^{\frac{v}{2\delta}(x - vt - p)}\right)^2 \text{ for } x \le vt + p, \quad c(x,y,t) = 0 \text{ for } x \ge vt + p.$$

The shift *p* defines the position of the front of the wave at t = 0 and is set to 0.2. Note that the problem is degenerate parabolic since  $\beta'(0) = +\infty$  and the solution takes the value of 0.

We perform the simulations on an unstructured triangular mesh; the initial one is given in Figure 7.1. The initial time step is T/2. We refine the space mesh by dividing each triangle regularly into four subtriangles and each time the space mesh is refined, the time step is divided by two. We define the Péclet number by Pe :=  $hv/\delta$ . The initial conditions are the values of the exact solution for t = 0at the midpoints of triangle edges. The boundary conditions are given in a similar way. The solution of the simulated problem is in fact only one-dimensional. We use this fact to test the performance of the numerical scheme that we propose for strongly irregular two-dimensional meshes. The case where the triangular mesh contains angles greater than  $\pi/2$  is similar to the case where the diffusion tensor is anisotropic: in both cases the discrete maximum principle is not necessarily satisfied (recall that this principle holds under Assumption (D), cf. Theorem 4.5). Hence we need to define the function  $\beta(c)$  for c < 0. To fulfill Assumptions (A1) and (A2), we set  $\beta(c) := -\beta(-c)$  for c < 0.

At each discrete time level, we have to solve the nonlinear system of algebraic equations given by (3.6a)-(3.6c). Since  $\beta'(0) = +\infty$  and since the solution takes the value 0, we cannot directly apply the Newton method for this purpose. The traditional finite element technique to overcome this difficulty consists in regularization (approximation of  $\beta$  by functions with bounded slope), cf. [8]. Another method, however applicable only when the discrete maximum principle holds, consists in perturbing the initial and boundary conditions so that all the values that the scheme works with were strictly positive (the problem is not anymore degenerate parabolic), see [39]. In our approach, we introduce new unknowns  $u_D^n = \beta(c_D^n)$  and rewrite the system of equations (3.6a)–(3.6c)



**Fig. 7.2** Approximate solution at t = 0.25,  $\delta = 0.01$ , r = 3

**Table 7.1** Number of refinements, number of time steps, number of unknowns, Péclet number, and computational times in min:sec for  $\delta = 0.05$ , 0.01, and 0.0001, respectively

Rf.	T. st.	Unkn.	$Pe_{\delta=0.05}$	$t_{\delta=0.05}$	$Pe_{\delta=0.01}$	$t_{\delta=0.01}$	$\text{Pe}_{\delta=0.0001}$	$t_{\delta=0.0001}$
1	4	88	4.56	0:01	22.80	0:01	2280.0	0:01
3	16	1504	1.14	0:16	5.70	0:15	570.0	0:11
5	64	24448	0.29	19:11	1.43	17:49	142.5	9:51

for these new unknowns, cf. [23]. We believe that this approach is advantageous for the following reasons: (i) There is no need to regularize the problem or to perturb the data (now  $[\beta^{-1}]'(0) = 0$ ); (ii) One can directly apply the Newton method to linearize the problem; (iii) The resulting matrices are diagonal for the part of the unknowns corresponding to the region where the concentration is zero. Indeed, on the step k of the linearization at time  $t_n$ , we approximate  $c_E^{n,k} = \beta^{-1}(u_E^{n,k}) \approx \beta^{-1}(u_E^{n,k-1}) + (\beta^{-1})'(u_E^{n,k-1})(u_E^{n,k} - u_E^{n,k-1})$ , which vanishes since  $\beta^{-1}(0) = (\beta^{-1})'(0) = 0$ . Let  $\{u_D^{n,k}\}_{D \in \mathcal{D}_h^{int}}$  be the solution vector on the step k. The linearization is terminated whenever

$$\left(\sum_{D\in\mathscr{D}_{h}^{int}} (u_{D}^{n,k} - u_{D}^{n,k-1})^{2}\right)^{\frac{1}{2}} / \left(\sum_{D\in\mathscr{D}_{h}^{int}} (u_{D}^{n,k})^{2}\right)^{\frac{1}{2}} \le 10^{-10}.$$

The bi-conjugate gradients stabilized method (Bi-CGStab), preconditioned by the LU incomplete factorization with drop tolerance  $10^{-3}$ , is used for the solution of the associated linear systems. The iterations were stopped whenever the relative residual decreased below  $10^{-10}$ .

We consider three values of  $\delta$ : 0.05, 0.01, and 0.0001. The number of refinements is r = 1,3, and 5 (r = 0 corresponds to the initial mesh). We refer to Table 7.1 for the number of unknowns, Péclet numbers, and computational times.



Fig. 7.3 Solution profiles for y = 0.5 and  $\delta = 0.01$ , at t = 0.5 (left) and at t = 0.75 (right)



Fig. 7.4 Solution profiles for y = 0.5 at t = 0.5,  $\delta = 0.05$  (left) and  $\delta = 0.0001$  (right)

For the finest meshes, there were up to 15 Newton steps necessary in the first iteration. This number then decreased to approx. 7 per time step. We can see the approximate solution for  $\delta = 0.01$  and r = 3 at t = 0.25 in Figure 7.2. We next give the profiles of approximate solutions in y = 0.5 for the different values of  $\delta$  and r in Figures 7.3 and 7.4. The profile in y = 0.5 is defined by all the calculated values  $c_D$  such that  $Q_D$  (the midpoint of the edge  $\sigma_D$  associated with the dual volume D) satisfies  $|Q_D - l_{0.5}| < 0.25$  for r = 1,  $|Q_D - l_{0.5}| < 0.08$  for r = 3, and  $|Q_D - l_{0.5}| < 0.02$  for r = 5, where  $l_{0.5}$  is the line y = 0.5.

We finally give some comments on the results. First, the scheme works easily for the given irregular mesh, which would not be possible with the standard finite volume method, cf. [23]. This irregularity (angles greater than  $\pi/2$ ) on the other hand causes the violation of the discrete maximum principle. However, this violation is only noticeable for the coarsest meshes (r = 0, 1, in power of  $10^{-3}$ ) and disappears with the refinement of the meshes. The scheme naturally works with negative values due to the appropriate definition of  $\beta(c)$  for c < 0. We remark that the negative values of the approximation that are visible in Figure 7.2 have no relation to the discrete maximum principle; they are only a consequence of a piecewise linear interpretation of the (non-negative) values  $c_D^n$ . The influence of unsuitable shapes of the elements is also visible in Figures 7.3 and 7.4—note the local fluctuations in the profiles for r = 1 and 3. This influence is however only because of the finite volume part of the scheme, which can be easily verified by considering a pure hyperbolic problem. Next, the local Péclet upstream weighting reduces the numerical diffusion of full upstream weighting to the amount exactly necessary to ensure the stability of the scheme. In particular, the coefficients  $\alpha_{D,E}^n$ given by (3.8) automatically increase with r. Moreover, the different values of these parameters for different dual sides of the mesh reflect the local ratio of the diffusion and convection fluxes (recall that e.g. for a dual side parallel with **v**, the flux of **v** through this side is zero). This numerical flux would be still more efficient for a problem where the ratio of v and  $\delta$  is not uniform over  $\Omega$ . Finally, precise approximation of realistic convection-dominated problems on fixed grids with the proposed scheme may still be expensive in terms of the computational cost. A local refinement strategy as those proposed in [37,38] would then be necessary.

7.2 A problem with an inhomogeneous and anisotropic diffusion-dispersion tensor

We consider here a problem with an inhomogeneous and anisotropic diffusiondispersion tensor and compare our scheme with three different ones.

The problem at hand is given by the equation (1.1) for  $\Omega = (0,2) \times (0,1)$  and T = 1 with

$$\begin{split} \beta(c) &= c + c^{\frac{1}{2}} \text{ for } c \geq 0, \\ F(c) &= \frac{1}{2} c^{\frac{1}{2}} \text{ for } c \geq 0, q = 0 \end{split}$$

and either

$$\mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ in } \boldsymbol{\Omega} \,, \quad \mathbf{v} = (3, 0) \text{ in } \boldsymbol{\Omega} \tag{7.1}$$

or

$$\mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ for } x < 1, \quad \mathbf{S} = \begin{pmatrix} 8 & -7 \\ -7 & 20 \end{pmatrix} \text{ for } x > 1,$$
$$\mathbf{v} = (3,0) \text{ for } x < 1, \quad \mathbf{v} = (3,12) \text{ for } x > 1.$$
(7.2)

Initial and Dirichlet or Robin boundary conditions are again given by the exact solution  $c(x, y, t) = e^{x}e^{y}e^{-t}/e^{3}$ . Note that in the case of the coefficients given by (7.2), the velocity field **v** as well as the flux of the solution given by  $-\mathbf{S}\nabla c + (c\mathbf{v})$  have a continuous normal trace across the discontinuity line x = 1.

We perform the simulations on refinements of the meshes A and B from Figure 7.5 and compare the scheme (3.6a)–(3.6c) (abbreviated as FV–NCFE) with the lowest-order Raviart–Thomas mixed finite element (MFE) method, with the combined finite volume–finite element (FV–FE) scheme, cf. [30], and finally, for the mesh A (where all angles are acute) and for coefficients (7.1) also with the pure cell-centered finite volume (FV) scheme, cf. [23,25]. Since we will only consider piecewise constant diffusion tensors, the two variants of our scheme coincide, see Remark 3.2. Finally, for the FV, FV–FE, and FV–NCFE schemes, we use the appropriate variant of the local Péclet upstream weighting (3.7), (3.8), whereas for



Fig. 7.5 Initial meshes A (top) and B (bottom)

Method $\setminus r$	0	1	2	3	4	5
PFV	0.02914	0.01159	0.00551	0.00276	0.00140	0.00070
PMFE	0.03480	0.01249	0.00558	0.00276	0.00139	0.00069
FV–FE	0.04892	0.01665	0.00693	0.00314	0.00149	0.00073
FV-NCFE	0.02642	0.01146	0.00554	0.00278	0.00140	0.00070

**Table 7.2** Discrete  $L^{\infty}(0,T;L^2(\Omega))$  relative errors, coefficients (7.1), mesh A

Method $\setminus r$	0	1	2	3	4	5
FV	0.04957	0.02428	0.01215	0.00608	0.00304	0.00152
MFE	0.02542	0.01099	0.00539	0.00273	0.00138	0.00070
FV–FE	0.13859	0.04922	0.01771	0.00655	0.00252	0.00102
FV-NCFE	0.03595	0.01495	0.00658	0.00306	0.00147	0.00072

**Table 7.3** Discrete  $L^{\infty}(0,T;L^2(\Omega))$  projection relative errors, coefficients (7.1), mesh A

mixed finite elements, we employ its centered form from [21], since the problem at hand is not convection-dominated.

Tables 7.2 and 7.3 give discrete relative and projection relative errors (see the definitions below) for all the compared schemes and up to five refinements of the original space-time grid, considering coefficients (7.1), mesh A, and Dirichlet boundary conditions. Similarly, tables 7.4 and 7.5 give the discrete relative and projection relative errors for the coefficients (7.2), mesh B, and Robin boundary conditions on x = 0 and Dirichlet boundary conditions otherwise. The discrete

 $L^{\infty}(0,T;L^{2}(\Omega))$  relative error is defined by

$$\max_{n \in \{1,2,...,N\}} \frac{\|c_h^n(\cdot) - c(\cdot,t_n)\|_{0,\Omega}}{\|c(\cdot,t_n)\|_{0,\Omega}}$$

where  $c_h^n$  is the piecewise linear approximate solution at time  $t_n$ : for the FV– FE and FV–NCFE schemes, we consider directly the resulting approximations, whereas for the FV and MFE schemes, a local postprocessing is used (we use the notation PFV and PMFE). We refer to [41] for the details. We define a discrete  $L^{\infty}(0,T;L^2(\Omega))$  projection relative error by

$$\max_{n \in \{1,2,\dots,N\}} \frac{\|\tilde{c}_h^n(\cdot) - \tilde{c}(\cdot,t_n)\|_{0,\Omega}}{\|c(\cdot,t_n)\|_{0,\Omega}}$$

where  $\tilde{c}_h^n$  is the piecewise constant approximate solution at time  $t_n$ . For the FV–FE and FV–NCFE schemes, we consider the solutions piecewise constant on the dual volumes, whereas for the FV and MFE scheme, we use the piecewise constant results on the triangles. The function  $\tilde{c}$  is given by the mean values of the exact solution c on the dual volumes for the combined schemes and on the triangles for the FV and MFE schemes. A quintic (7-point) numerical integration formulae was used for the approximate evaluation of the error. Finally, since in this case the solution does not take the value 0, directly the Newton method was used for the linearization (with the stopping criterion  $10^{-8}$ ).

In the first tested case (constant coefficients), the discrete  $L^{\infty}(0,T;L^2(\Omega))$  relative errors were comparable for all the schemes on the finest mesh. For the discrete  $L^{\infty}(0,T;L^2(\Omega))$  projection relative error, there are some minor differences—the lowest error is produced by the mixed finite element method and the highest by the finite volume one. In the second tested case (discontinuous coefficients), the differences are more important. In what concerns the discrete  $L^{\infty}(0,T;L^2(\Omega))$  errors, the FV–NCFE scheme gave much better results than the FV–FE scheme. One of the possible reasons is that the latter scheme employs the arithmetic average of the heterogeneities associated with the triangles. The results of the FV–NCFE scheme were on the other hand comparable to that given by the elementwise linear postprocessed solution of the MFE scheme. Again the differences are more important for the  $L^{\infty}(0,T;L^2(\Omega))$  projection error. Finally, the experimental order of convergence for all the compared schemes was  $O(h, \Delta t)$  for fine meshes and a little bit better for coarser meshes.

The computational cost of the different schemes was also compared in [41]. In general, the FV–FE scheme requires much less CPU time than the FV–NCFE one, since its unknowns are associated with vertices, whereas in the FV–NCFE scheme, the unknowns are associated with edges. However, the higher precision of the FV–NCFE scheme in the tested cases was important enough to persist to the "efficiency graph" (plotting the error against the CPU time), especially for problems with discontinuous coefficients and inhomogeneous and anisotropic diffusion tensors. The mixed finite element method in its original formulation requires quite an increased CPU time. However, considering its equivalent finite volume form [43] where the degrees of freedom are only associated with the triangles, it is also very competitive, although not as fast as the FV scheme.

As a conclusion, we find that the FV–NCFE scheme proposed and studied in this paper represents an easy extension of the finite volume method to general

Method $\backslash r$	0	1	2	3	4	5
PMFE 0	).02608	0.00761	0.00259	0.00110	0.00053	0.00026
FV-FE 0	).03961	0.01345	0.00537	0.00238	0.00111	0.00054
FV-NCFE 0	).01990	0.00680	0.00293	0.00143	0.00072	0.00036

**Table 7.4** Discrete  $L^{\infty}(0,T;L^2(\Omega))$  relative errors, coefficients (7.2), mesh B

Method $\setminus r$	0	1	2	3	4	5
MFE	0.00821	0.00389	0.00199	0.00102	0.00052	0.00027
FV–FE	0.13895	0.04848	0.01713	0.00619	0.00230	0.00089
FV-NCFE	0.03122	0.01210	0.00475	0.00197	0.00087	0.00040

**Table 7.5** Discrete  $L^{\infty}(0,T;L^2(\Omega))$  projection relative errors, coefficients (7.2), mesh B

meshes and inhomogeneous and anisotropic diffusion tensors, which is simpler, more straightforward, and more finite volume-like than the mixed finite element method, but gives comparable results.

## 8 Appendix: Technical lemmas

We give here some technical lemmas that were needed in paper.

Lemma 8.1 Let us consider the elliptic problem

$$-\nabla \cdot (\mathbf{S}\nabla p) = q \quad in \ \Omega, \tag{8.1a}$$

$$p = 0 \quad on \ \partial \Omega \,, \tag{8.1b}$$

where  $q \in L^2(\Omega)$ . Then the stiffness matrix for the Lagrange multipliers of the hybridization of the lowest-order Raviart–Thomas mixed finite element method on the simplicial mesh  $\mathcal{T}_h$  has the form

$$\mathbb{M}_{D,E} = -\sum_{K \in \mathscr{T}_h} (\mathbf{S}_K \nabla \varphi_E, \nabla \varphi_D)_{0,K} \qquad D, E \in \mathscr{D}_h^{int},$$
(8.2)

where

$$\mathbf{S}_{K} = \left(\frac{1}{|K|} \int_{K} \mathbf{S}^{-1} \, \mathrm{d}\mathbf{x}\right)^{-1} \qquad \forall K \in \mathscr{T}_{h}.$$
(8.3)

*Proof* The hybridization of the lowest-order Raviart–Thomas mixed finite element method for the problem (8.1a)–(8.1b) reads (cf. [12, Section V.1.2]): find  $\mathbf{u}_h \in \mathbf{V}_h$ ,  $p_h \in \Phi_h$ , and  $\lambda_h \in \Lambda_h$  such that

$$\sum_{K \in \mathscr{T}_h} \left\{ (\mathbf{S}^{-1} \mathbf{u}_h, \mathbf{v}_h)_{0,K} - (\nabla \cdot \mathbf{v}_h, p_h)_{0,K} + \langle \mathbf{v}_h \cdot \mathbf{n}, \lambda_h \rangle_{\partial K} \right\} = 0 \qquad \forall \mathbf{v}_h \in \mathbf{V}_h, (8.4a)$$

$$-\sum_{K\in\mathscr{T}_h} (\nabla \cdot \mathbf{u}_h, \phi_h)_{0,K} = -(q, \phi_h)_{0,\Omega} \qquad \forall \phi_h \in \Phi_h,$$
(8.4b)

$$\sum_{K \in \mathscr{T}_h} \langle \mathbf{u}_h \cdot \mathbf{n}, \mu_h \rangle_{\partial K} = 0 \qquad \forall \mu_h \in \Lambda_h \,. \tag{8.4c}$$

Here,  $\mathbf{V}_h$  is the space of elementwise linear vector functions such that  $\mathbf{u}_h \in \mathbf{V}_h$  satisfies  $\mathbf{u}_h|_K = (a_K + d_K x, b_K + d_K y)$  if d = 2 and  $\mathbf{u}_h|_K = (a_K + d_K x, b_K + d_K y, c_K + d_K z)$  if d = 3 for all  $K \in \mathcal{T}_h$ ,  $\Phi_h$  is the space of elementwise constant scalar functions, and  $\Lambda_h$  is the space of sidewise constant scalar Lagrange multipliers. For all  $D \in \mathcal{D}_h$ , we denote  $\lambda_h|_{\sigma_D}$  by  $\lambda_D$  and require  $\lambda_D = 0$  for all  $D \in \mathcal{D}_h^{ext}$ . We now extend the ideas of [14], where the tensor **S** is supposed piecewise constant on  $\mathcal{T}_h$ .

Let us set  $\tilde{\lambda}_h := \sum_{D \in \mathscr{D}_h} \lambda_D \varphi_D$ . Using (3.13), we have

$$\sum_{\sigma_D \in \mathscr{E}_K} \lambda_D |\sigma_D| \mathbf{n}_{\sigma_D} = |K| \sum_{\sigma_D \in \mathscr{E}_K} \lambda_D \nabla \varphi_D|_K = |K| \nabla \tilde{\lambda}_h|_K.$$

Then denoting the unit coordinate vectors as  $\mathbf{e}_i$  and taking, respectively,  $\mathbf{v}_h = \mathbf{e}_i$  in  $K, 1 \le i \le d, \mathbf{v}_h = 0$  otherwise as the test functions in (8.4a), we come to

$$\int_{K} \mathbf{S}^{-1} \mathbf{u}_{h} \, \mathrm{d}\mathbf{x} + |K| \, \nabla \tilde{\lambda}_{h}|_{K} = 0 \qquad \forall K \in \mathscr{T}_{h} \, .$$

Next we note that the stiffness matrix does not depend on q and hence we can pose q = 0. Considering  $\phi_h = 1$  on K and zero otherwise in (8.4b), this yields  $d_K = 0$  for all  $K \in \mathcal{T}_h$ . Hence  $\mathbf{u}_h|_K = -\mathbf{S}_K \nabla \tilde{\lambda}_h|_K$  with  $\mathbf{S}_K$  given by (8.3). It now suffices to substitute this into (8.4c) to obtain a system for the Lagrange multipliers  $\lambda_D$ ,  $D \in \mathcal{D}_h^{int}$ , with the matrix given by (8.2).  $\Box$ 

**Lemma 8.2** Let us consider the function B(s),  $s \in \mathbb{R}$ ,  $B(s) = \beta(s)s - \int_0^s \beta(\tau) d\tau$ , with  $\beta$  satisfying Assumption (A1). Then  $B(s) \ge s^2 c_\beta/2$  for all  $s \in \mathbb{R}$ .

*Proof* Let us first consider a given  $s \ge 0$ . We then have for each h > 0

$$\frac{B(s+h)-B(s)}{h} = \frac{\beta(s+h)-\beta(s)}{h}s + \beta(s+h) - \frac{1}{h}\int_{s}^{s+h}\beta(\tau)\,\mathrm{d}\tau$$

This gives, using the fact that  $\beta(s+h) - \beta(s) \ge c_{\beta}h$ , which follows from Assumption (A1), and the continuity of  $\beta$ 

$$\liminf_{h\to 0^+} \frac{B(s+h) - B(s)}{h} \ge c_\beta s$$

Hence, using the fact that B(0) = 0 and that  $s^2 c_\beta/2 = 0$  for s = 0, we have  $B(s) \ge s^2 c_\beta/2$  for all  $s \ge 0$ . The proof for s < 0 proceeds similarly.  $\Box$ 

**Lemma 8.3** Let  $\beta$  satisfy Assumption (A2). Then  $[\beta(s)]^2 \leq 2C_{\beta}^2 + 4L_{\beta}^2P^2 + 4L_{\beta}^2s^2$  for all  $s \in \mathbb{R}$ .

*Proof* If  $s \in [-P, P]$ , the assertion of the lemma is trivially satisfied, since by Assumption (A2),  $|\beta(s)| \le C_{\beta}$ . If s > P, then using the Lipschitz continuity of  $\beta$  on  $[P, +\infty)$ , one has

$$\beta(s) = \beta(P) + \beta(s) - \beta(P) \le \beta(P) + L_{\beta}(s - P)$$

and similarly for s < -P. Thus, using the inequality  $(a \pm b)^2 \le 2(a^2 + b^2)$  and  $|\beta(\pm P)| \le C_\beta$ , one has, for |s| > P,

$$[\beta(s)]^2 \le 2C_{\beta}^2 + 4L_{\beta}^2P^2 + 4L_{\beta}^2s^2. \quad \Box$$

**Lemma 8.4** Let  $\Omega \subset \mathbb{R}^p$ , p > 1, be an open bounded set,  $\{a_n, n \in \mathbb{N}\}$  a sequence of functions from  $L^2(\Omega)$ , defined by zero on  $\mathbb{R}^p \setminus \Omega$ ,  $h_n$  a sequence of non-negative real values with  $\lim_{n\to\infty} h_n = 0$ , and C > 0. Let the functions  $a_n$  satisfy

$$\int_{\Omega} \left( a_n(\mathbf{x} + \boldsymbol{\eta}) - a_n(\mathbf{x}) \right)^2 d\mathbf{x} \le C |\boldsymbol{\eta}| + h_n \qquad \forall \boldsymbol{\eta} \in \mathbb{R}^p, \, \forall n \in \mathbb{N}.$$
(8.5)

Then

$$\forall \boldsymbol{\varepsilon} > 0 \quad \exists \boldsymbol{\zeta} > 0 \quad \forall \boldsymbol{\eta} \in \mathbb{R}^{p}, \, |\boldsymbol{\eta}| < \boldsymbol{\zeta} \quad \forall n \in \mathbb{N} \quad \int_{\Omega} \left( a_{n}(\mathbf{x} + \boldsymbol{\eta}) - a_{n}(\mathbf{x}) \right)^{2} \mathrm{d}\mathbf{x} \leq \boldsymbol{\varepsilon} \,.$$

$$(8.6)$$

*Proof* Let us consider a fixed  $\varepsilon > 0$ . Let  $n_0$  be such that  $\forall n > n_0$ ,  $|h_n| < \varepsilon/2$ . The continuity in mean of the functions  $a_1, \ldots, a_{n_0}$  implies

$$\int_{\mathbb{R}^p} \left( a_i(\mathbf{x} + \boldsymbol{\eta}) - a_i(\mathbf{x}) \right)^2 d\mathbf{x} \longrightarrow 0 \text{ as } |\boldsymbol{\eta}| \to 0 \qquad \forall i \in \{1, \dots, n_0\},$$

or, more precisely,

$$\forall i \in \{1, \dots, n_0\} \quad \forall \varepsilon^* > 0 \quad \exists \zeta_i^* > 0 \quad \forall \eta^* \in \mathbb{R}^p, \, |\eta^*| < \zeta_i^* \\ \int_{\mathbb{R}^p} \left( a_i(\mathbf{x} + \eta^*) - a_i(\mathbf{x}) \right)^2 \mathrm{d}\mathbf{x} \le \varepsilon^* \,.$$
(8.7)

We set  $\varepsilon^* = \varepsilon$  in (8.7) and define  $\zeta^* := \min_{i=1,...,n_0} \zeta_i^*$ . Since  $n_0 < \infty$ ,  $\zeta^* > 0$ . It is finally enough to choose

$$\zeta = \min\left\{\zeta^*, \frac{\varepsilon}{2C}\right\}.$$

Indeed, for  $n < n_0$ , estimate (8.6) is valid due to (8.7). For  $n > n_0$ , (8.5) and the fact that  $|h_n| < \varepsilon/2$  yields the assertion of the lemma.  $\Box$ 

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