Analysis of a model for precipitation and dissolution coupled with a Darcy flux

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1. Introduction

The study of reactive flow in porous media is of particular relevance in several applications ranging from geochemical reactions in sedimentary basins [3,4], kerogen degradation and expulsion in oil reservoirs [23], groundwater contamination and remediation processes [21], biomedical applications such as drug release from drug eluting devices [17,10,2].

These processes can be characterized by the presence of phenomena such as adsorption that, at the macroscale, can be effectively modeled by discontinuous reaction terms. The process of crystal precipitation/dissolution, which is the subject of this work, is usually modeled with a discontinuous dissolution rate

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to take into account that the dissolution takes place only if the crystal concentration is above a given value. Thus, the discontinuity depends on the solution itself. Therefore, to prove the existence of a solution, and to determine its behavior at the discontinuity, we have to resort to Filippov theory [9]. When the trajectory of the solution reaches the surface of discontinuity, in the phase space it can cross the surface or slide onto it until a suitable exit condition is met. This class of problems may be interpreted as differential inclusions: a recent review on their numerical treatment, in the context of ODEs, is found in [8].

In this work we consider the simplified, yet realistic model of precipitation and dissolution proposed in [25] whose numerical treatment has been considered in [15,14]. The model is defined at Darcy scale and describes the dissolution and precipitation process leading to the formation/degradation of crystals inside a porous matrix, where the reactants are advected by a given velocity field. We consider here a variable velocity field described by the coupling with a Darcy model where porosity and permeability are linked to the crystal concentration by an empirical law. The model involves a non-linear discontinuous reaction term that describes the fact that the dissolution process starts only when the concentration of the reactants reaches a certain critical value, and is cast as a differential inclusion.

In [26] and [16] rigorous models for crystal dissolution and precipitation in a porous medium, in which the amount of precipitate does affect the pore structure, are developed, starting from two-dimensional micro-scale models with free boundaries and using upscaling techniques. These models provide the precise dependency of the porosity and permeability on the amount of precipitate. The simplified coupled model studied here retains the main mathematical difficulties of the coupling laws introduced in [26] and [16].

In [20] a model in which reactive transport of a solute coupled to unsaturated Darcy flow, obtained by solving the Richards equation for water flux and water saturation, is considered, and an Euler implicit-mixed finite element scheme is analyzed. In that study, the focus is on the solute transport and reaction, and the convergence of the scheme is shown assuming that at each time level the solute concentration does not influence the water flow quantities.

In [19] an Euler implicit-mixed finite element scheme for multicomponent transport and flow is proposed, with a dependence of the porosity and the permeability on the concentrations, deduced from the models introduced in [26]. In this study the necessary estimates to show the convergence of the scheme are deduced only for the case of constant porosity.

We focus here on the analysis of the fully coupled problem, showing for the first time its well posedness, as well as the convergence to its weak solution of a particular finite element approximation. This result is an important extension of that provided in the quoted references, where the velocity field was a given datum or was not affected by the solute transport and reaction, and where a regularization approach was followed.

The main difficulties we had to face are the following:

- to show regularity and non-degeneracy of the Darcy field, which is described by a Darcy law with discontinuous permeability and forcing term;
- to bound the nonlinear coupling terms between the Darcy field and the cation concentration;
- to obtain energy estimates for the Darcy velocity and pressure that guarantee the convergence of a sequence of approximations to the solution.

We show some numerical results that underline the fact that by using a method that captures the discontinuity accurately we get sharper dissolution fronts than regularization methods. For the sake of brevity, we have omitted the details of the numerical techniques based on event-driven methods [6] that we have employed, which are the subject of a forthcoming work.

The paper is organized as follows: in Section 2 we outline the mathematical model for dissolution–precipitation, which is taken from [15], and the coupling with a Darcy velocity field. We first give the main result of uniqueness and regularity of the solution of the coupled problem. The existence of solutions is proved in Section 2.5, via a Faedo–Galerkin approach. We construct a finite element approximation and we prove that the limit solution exists and coincides with that of the original differential problem. The final section is devoted to the illustration of a numerical result that shows the effectiveness of the model.

2. A simplified model of dissolution and precipitation

We introduce a model that describes the flow in a porous medium with ions dissolved in water that move under the action of transport and diffusion and precipitate in a crystal form [25]. We model the problem at the Darcy scale: the medium is a continuum, and the pores and solid particles are homogenized on a reference volume element. We are interested in studying the interaction of transport and diffusion, with the chemical reactions that determine the process of ion (anion and cation) precipitation and dissolution. These processes transform the dissolved ions into immobile solid species, with the consequent formation/dissolution of crystals.

2.1. Nomenclature

With $\Omega \subset \mathbb{R}^2$ we indicate the domain of the problem, occupied by the porous medium. The domain is open and polygonal, with boundary $\partial\Omega = \Gamma = \Gamma_D \cup \Gamma_N$. To obtain uniqueness and regularity results we may need to impose further restrictions later on. With $T > 0$ we denote a given final time. We further define

$$\Omega^T = (0,T] \times \Omega, \Gamma^T_{D,N} = (0,T] \times \Gamma$$

and we indicate with $L^p(\Omega)$, $H^m(\Omega)$ and $L^p((0,T);V)$ the usual Banach and Sobolev spaces and spaces with values in Sobolev spaces [1], for a $p \in [1,\infty]$ and $m \in \mathbb{N}$. While, $\boldsymbol{H}_{\mathrm{div}}(\Omega) = \{\mathbf{v} \in [L^2(\Omega)]^2,\ \mathrm{div}\,\mathbf{v} \in L^2(\Omega)\}$. With $\|\cdot\|$ we indicate the $L^2(\Omega)$ norm.

For a function $u : \Omega^T \to \mathbb{R} : u = u(t,\mathbf{x})$ we set $u(t) : \Omega \to \mathbb{R} : u(t)(\mathbf{x}) = u(t,\mathbf{x})$, and analogously for vector functions.

Furthermore, $C, D, E, \ldots$ denote throughout generic positive constants independent of the unknown variables or the discretization parameters, the value of which might change from line to line.

2.2. The model

We use the simplified model considered in [15,14], here briefly recalled for the convenience of the reader. While reactions usually take place between various cations and anions, this simplified model considers only one mobile species, whose mass concentration is denoted by u. The mass concentration of the (immobile) precipitate is denoted by v.

The following adimensionalized problem for the evolution of the reactant u is derived from the mass conservation principle and the chemical balance dynamics [15,14]:

$$\begin{cases} \dfrac{\partial}{\partial t}(u+v) - \mathrm{div}\big(\nabla u - \mathbf{q}u\big) = 0 \quad \text{in} \quad \Omega^T, \\ u = g \quad \text{in} \quad \Gamma^T_D, \\ \nabla u \cdot n = h \quad \text{in} \quad \Gamma^T_N, \\ u = u_0 \quad \text{in} \quad \Omega \quad \text{for} \quad t = 0, \end{cases} \tag{1}$$

where g and h are given data, and $\mathbf{q} \in \boldsymbol{H}_{\mathrm{div}}(\Omega)$ is a velocity field governed by Darcy's law. The coupling with the Darcy problem is described later. The diffusion coefficient has been taken equal to 1 for simplicity.

System (1) is coupled with the adimensionalized equation for the precipitate that reads

$$\begin{cases} \dfrac{\partial}{\partial t} v = r(u) - H(v) & \text{in} \quad \Omega^T, \\ v = v_0 \quad \text{in} \quad \Omega \quad \text{for} \quad t = 0, \end{cases} \tag{2}$$

where $r(u)$ and $H(v)$ are the production and dissolution rates, respectively, so that the rate of change in the precipitate concentration is the net result of the process of precipitation and dissolution. It is assumed that $r : \mathbb{R} \to [0, \infty)$ is locally Lipschitz continuous with the following properties:

$$\begin{cases} r(u) = 0 \quad \text{for } u \leq 0, \\ r(u) \quad \text{monotonically increasing for} \quad u \geq 0, \\ r(1) = 1. \end{cases} \tag{3}$$

Here, $u = 0$ and $u = 1$ are two limiting values. The former sets the minimal concentration required to activate the reaction. The latter limits the maximal (adimensional) reaction rate to one.

Remark 1. A more general assumption for (3) is given by

$$\begin{cases} r(u) = 0 \quad \text{for } u \leq u_* \quad \text{with } 0 \leq u_* < 1, \\ r \quad \text{monotonically increasing for} \quad u \geq u_*, \\ r(u^*) = 1 \quad \text{for } u_* < u^*. \end{cases}$$

Note that, if $r(u) = u^n$, $n \in \mathbb{N}^+$ (in [15] $r(u) = u^2$, as given by the mass balance law), then $u_* = 0$, i.e. $r(u) = \text{Proj}_{\mathbb{R}^+}(u^n)$, and $u^* = 1$.

The dissolution rate is described by the Heaviside graph

$$H(v) = \begin{cases} 0 \quad \text{for} \quad v < 0, \\ [0,1] \quad \text{for} \quad v = 0, \\ 1 \quad \text{for} \quad v > 0, \end{cases}$$

which is a set-valued function. Thus, the equal symbol in equations (1) and (2) should in fact be replaced by an inclusion symbol. Following [14,15], we choose the selection

$$H(v) = \min\{1, r(u)\} \quad \text{if } v = 0. \tag{4}$$

With this choice the dissolution rate becomes a discontinuous function, depending on u and v.

Remark 2. With reference to Remark 1, since here $u^* = 1$ and all the results below will be obtained for boundary and initial concentrations u_0 and v_0 with values below 1, as it will be clear later only a net effect of dissolution will be encountered and no precipitation will be possible in equation (2). In the more general case when the initial data $u_0 > u^*$ also precipitation is encountered. Nevertheless, the difficulty in the model remains the same.

If $u = 1$ everywhere at a given time t^*, then the system is in equilibrium for $t > t^*$, i.e. no precipitation or dissolution occur, since the precipitation rate is balanced by the dissolution rate regardless of the value of v. Analogously, if $v = 0$ everywhere at a given time t^*, then the system is in equilibrium for $t > t^*$. This model describes the fact that there is a threshold value for the concentration of the reactant above which dissolution starts.

2.3. Analysis of the differential inclusion problem

Contrary to what has been done in [15] we do not regularize the dissolution term. Since it is a jump discontinuous function, the solution may not be everywhere differentiable in $(0, T)$. We need then to exploit some results on finite dimensional Ordinary Differential Equations with Discontinuous Right Hand Side (ODE with DRH) and adopt special techniques for the numerical solution of the problem.

Let us introduce a family of finite dimensional subspaces V_h of $H^1(\Omega)$ such that $H^1(\Omega)$ is a Hilbertian sum of the V_h. Let us denote by $P_h : L^2(\Omega) \to V_h$ the projection operator, and by $u_h = P_h u,\ v_h = P_h v$. Problem (2) becomes: at any time t, given u_h, find v_h such that

$$\begin{cases} \dfrac{\partial}{\partial t} v_h \in r(u_h) - H(v_h) & \text{in} \quad \Omega^T, \\ v_h = P_h[v(0)] & \text{in} \quad \Omega \quad \text{for} \quad t = 0, \end{cases} \tag{5}$$

where we have supposed that $v(0) \in L^2(\Omega)$.

Lemma 1. *System (5) has a unique solution.*

Proof. The proof is based on the fact that (5) represents a family of non-autonomous finite dimensional inclusion problems on the parameter h. For any $\mathbf{x} \in \Omega$ this problem is isomorphic to $\dot{\mathbf{z}} \in F(t, \mathbf{z}(t)),\ t \in [0, T],\ z(0) = z_0$ with $z : \mathbb{R} \to \mathbb{R}^n$, $\mathbf{F} : \mathbb{R} \times \mathbb{R}^n \to 2^{\mathbb{R}^n}$, $n \in \mathbb{N}$. An existence and uniqueness result for this inclusion problem is expressed in the following theorem:

Theorem 1. *Let the set valued map $F = F(t, \mathbf{z})$ satisfy the following conditions:*

1. *the sets $F(t, \mathbf{z})$ are closed and convex,*
2. *the map $F(\cdot, \mathbf{z})$ is Lipschitz continuous (measurability is only required for existence) and the map $F(t, \cdot)$ is Upper Semi-Continuous (USC), i.e. the closure of the set $\{F(t, \mathbf{z}) |\ \|\mathbf{z} - \mathbf{z}_0\| < \delta\}$, $\delta > 0$, is compact $\forall \mathbf{z}_0 \in \mathbb{R}^n$,*
3. *$F(t, \mathbf{z})$ satisfies a growth condition: $\forall \mathbf{y} \in F(t, \mathbf{z})\ \exists k(t) > 0$ and $a(t) \mid \|\mathbf{y}\| \leq k(t)\|\mathbf{z}\| + a(t)$, for all $\mathbf{z} \in \mathbb{R}^n$.*

Then there is an absolutely continuous solution to the differential inclusion, for every $\mathbf{z}_0 \in \mathbb{R}^n$. If moreover the map $F(t, \mathbf{z})$ is One-Sided Lipschitz Continuous (OSLC), i.e. if there exists a constant $L(t)$ such that for every $\mathbf{z}_1$, $\mathbf{z}_2$, and for every $\mathbf{y}_1 \in F(t, \mathbf{z}_1)$ and $\mathbf{y}_2 \in F(t, \mathbf{z}_2)$,

$$(\mathbf{z_1} - \mathbf{z_2}, \mathbf{y_1} - \mathbf{y_2}) \leq L(t)\|\mathbf{z_1} - \mathbf{z_2}\|^2,$$

then the solution is unique. Analogous results exist at the continuous level, given by the Hille–Yosida theory for maximal monotone nonlinear operators.

The proof may be found in [9]. The set-valued map $H(v_k)$ has the following properties:

1. it is convex, compact and maximal monotone (indeed it can be characterized as the subdifferential of a convex function);
2. it satisfies the growth condition, with $k = a = 1$ (in particular it satisfies a boundedness condition with $k = 0$);
3. it is USC and the term $-H(v_k)$ is OSLC with $L = 0$ (due to the monotonicity property of $H(v_k)$).

Therefore, according to Theorem 1, and using the properties of the map $r(\cdot)$ and the time regularity of the solutions u_h which will be given below, problem (5) admits a unique absolutely continuous solution. □

To integrate system (5) at discrete level, we have to select an element of the set $H(0)$ when $v_h = 0$. This selection should coincide with the prescription introduced in equation (4) at the continuous level, i.e.

$$H(v_h) = \min\{1, r(u_h)\} \quad \text{if } v_h = 0. \tag{6}$$

We use the results coming from the theory of Filippov [9], and exploited for the numerical solution in [6,7], in the context of *event-driven* methods. The reader may refer to the quoted references for details, which we do not report here for the sake of brevity.

2.4. Coupling with a Darcy model

We consider the coupling of the precipitation–dissolution model (1)–(2) with the Darcy equations for a single phase fluid with constant density (water, in the case of our interest). Namely, the advection velocity field for the cation transport process in (2) is the solution of the problem for $\mathbf{q}$ and p given by

$$\begin{cases} \dfrac{\partial \phi}{\partial t} + \operatorname{div} \mathbf{q} = 0 \quad \text{in } \Omega^T, \\ \mathbf{q} = -\dfrac{k(\phi)}{\mu} \nabla p \quad \text{in } \Omega^T, \\ p = p_D \quad \text{on } \Gamma_D^T, \\ \mathbf{q} \cdot \mathbf{n} = \eta \quad \text{on } \Gamma_N^T, \end{cases} \tag{7}$$

where we have indicated the essential and the natural boundary conditions with data η and p_D, respectively. Here ϕ is the porosity, $\mathbf{q}$ is the macroscopic velocity, p is the fluid pressure, $\mu > 0$ is the dynamic viscosity and k is a scalar permeability.

The Darcy model is coupled to the cation dynamics by the fact that the precipitation and dissolution processes influence the porosity and thus also the permeability of the medium. In particular, with the increase of the precipitate concentration there is a consequent reduction of porosity; an empirical law for the variation of porosity with varying precipitate concentration is given by [12]

$$\frac{d\phi}{dt} = -\frac{\partial v}{\partial t}. \tag{8}$$

At each time we have $\phi = \phi_0 - v$, with ϕ_0 a constant which we take, for the sake of simplicity, equal to 1. The permeability coefficient is modeled as a positive Lipschitz continuous function of porosity. A possible empirical law is [12]

$$k(\phi) = (\phi)^2 \rightarrow k(\phi(v)) = (\phi_0 - v)^2 = (1 - v)^2, \tag{9}$$

for $v \in [0, 1]$.

Remark 3. In [26] and [16] rigorous models for crystal dissolution and precipitation in a porous medium, in which the amount of precipitate does affect the pore structure, are developed, starting from two-dimensional micro-scale models with free boundaries and using upscaling techniques. These models provide the precise dependency of the porosity and permeability on the amount of precipitate, in terms of the thickness of the layer of precipitated crystal around the grain boundaries, where the porosity enters also in the mass balance equations for the solute and the precipitate.

Here, starting from the model of precipitation and dissolution (1) and (2), proposed in [25], coupled to the Darcy equations (7) through the empirical laws (8) and (9), we obtain a simplified coupled model, where the porosity does not enter explicitly into the reactive transport equations. However the model retains the main mathematical difficulties of the coupling laws introduced in [26] and [16].

Indeed, using (8) and introducing the porosity weight factor in the mass balance equations for the solute and the precipitate (1) and (2), we would obtain the following adimensionalized reactive transport equation:

$$(1-v)\partial_t u - \operatorname{div}\big(\nabla u - \mathbf{q}u\big) = (1-v)(u-1)[r(u) - H(v)], \tag{10}$$

which, coupled to the Darcy equations (7), gives a similar model to that introduced in [20]. Note that, for $0 \le v < 1,\ 0 \le u \le 1$, the reactive transport model (10) retains the same mathematical properties as the simplified model described by (1) and (2).

In order to avoid numerical difficulties linked with the degeneracy of the Darcy equations at the discrete level, as will be explained in Section 2.5, we introduce the following regularization of the permeability coefficient:

$$k_\epsilon(v) := k(\min\{1-\epsilon, v\}),\ \epsilon > 0.$$

Note that $k_\epsilon(v)$ is a Lipschitz continuous function for $v > 0$. For the analysis we consider $\eta = 0,\ \ g = 0$ and $h = 0$. We also assume throughout that $|\Gamma_D| > 0$. Let us define the following functional spaces: $\mathcal{U} := \{u \in L^2((0,T); H_0^1(\Omega)) : \partial_t u \in L^2((0,T); H^{-1}(\Omega))\}$, $\mathcal{V} := \{v \in H^1([0,T]; L^2(\Omega))\}$, $\mathcal{Q} := L^2(\Omega^T)$, $\mathcal{Z} := L^2((0,T); \boldsymbol{H}_{\operatorname{div}}(\Omega))$.

The weak formulation of the coupled problem reads:

Problem $\mathbf{P_2}$. For a given $\epsilon > 0$, find $(\mathbf{q}, p) \in \mathcal{Z} \times \mathcal{Q}$ and $(u, v) \in \mathcal{U} \times \mathcal{V}$, with $(u(0), v(0)) = (u_0, v_0)$, such that for all $(\boldsymbol{\tau}, \psi) \in \boldsymbol{H}_{\operatorname{div}}(\Omega) \times L^2(\Omega)$ and $(\omega, \theta) \in H_0^1 \times L^2(\Omega)$,

$$\begin{cases} \big(\frac{\mu}{k_\epsilon(v)}\mathbf{q}(t), \boldsymbol{\tau}\big) - (p(t), \operatorname{div}\boldsymbol{\tau}) = -(p_D, \boldsymbol{\tau}\cdot\mathbf{n})_{\Gamma_D}, \\ (\operatorname{div}\mathbf{q}(t), \psi) = (-\frac{\partial\phi(v)}{\partial t}, \psi) = (\partial_t v(t), \psi), \\ (\partial_t u(t), \omega) + (\nabla u(t), \nabla\omega) - (\mathbf{q}(t)u(t), \nabla\omega) \in (H(v(t)) - r(u(t)), \omega), \\ (\partial_t v(t), \theta) \in (r(u(t)) - H(v(t)), \theta), \end{cases} \tag{11}$$

for $t \in (0, T)$, with $H(v)$ satisfying the selection (4), $u(0) = u_0 \in L^2(\Omega)$ and $v(0) = v_0 \in L^2(\Omega)$.

Our main results are stated in the following two theorems.

Theorem 2. *Let Ω be a convex polygonal domain, and let $p_D \in H^{1/2}(\Gamma_D)$. Assume moreover that $0 \le u_0 \le 1$ and $0 \le v_0 < 1$. Then there exists a solution of* (11)*.*

This theorem will be proven in the next section through the convergence result of the fully discrete problem employing the Euler method for time integration.

Theorem 3. *Under the same hypothesis of Theorem 2 and the additional assumptions that Ω is a convex polygonal domain with convex angles given by a rational fraction of π (for example $\Omega = [-L, L] \times [-l, l]$), and that the Dirichlet and Neumann data are imposed on whole polygon edges, if $\mathbf{q} \in [L^\infty(\Omega)]^2$, then the solution of* (11) *is unique.*

Remark 4. The hypothesis of $\mathbf{q} \in [L^\infty(\Omega)]^2$ is perfectly reasonable due to the additional assumption of Theorem 3. Indeed, it is possible to prove, by using some results on the regularity of elliptic equations with rough coefficients in polygonal domains, that $p \in C^{0,\beta}(\bar{\Omega})$, for a $\beta \in (0, 1)$ (see [13], Chapter 14, in particular Theorem 14.2.1, for the regularity on compact subsets of Ω; see [11], Chapter 6, in particular result $(6, 4, 2, 1)$, for the regularity near the corner of the domain, supposing that v_0 has no discontinuity near the corners; see also [22]). This means that p is almost everywhere a Lipschitz function, and, together with the boundedness of $k_\epsilon(v)$, this provides the wanted regularity for the velocity. For the sake of brevity we omit the proof.

Remark 5. By compactness arguments it may be shown that if, in addition to the stated hypotheses, $u_0 \in H_0^1(\Omega)$, then $u \in C^0([0, T]; H_0^1(\Omega)) \cap L^2(0, T; H^2(\Omega))$ is a global strong solution of (11).

In order to proceed with the proof of Theorem 3 we need the following

Lemma 2. *Under the stated hypotheses on the initial data and on k_ϵ, $0 \le v(t) < 1$ and $0 \le u(t) \le 1$ a.e. in $L^2(\Omega)$ for all $t \in (0, T]$, independently of ϵ, and $\mu/k_\epsilon(v(t)) \in L^\infty(\Omega)$ and is positive. The solution u belongs to $L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H_0^1(\Omega))$, $v \in L^\infty(0, T; L^2(\Omega))$, $\mathbf{q} \in \boldsymbol{H}_{\mathrm{div}}(\Omega)$, $p \in L^2(\Omega)$, $\partial_t v(t) \in L^\infty(\Omega)$ and $\partial_t u(t) \in L^2(0, T; H^{-1}(\Omega))$.*

Proof. Let us set $R(u, v) = r(u) - H(v)$. We may note that

- $R(u, v) \ge 0$ if $v \le 0$, for all u;
- $R(u, v)$ is either 0 or -1 if $u \le 0$;
- $R(u, v) \le 0$ if $v \ge 0$ and $0 \le u \le 1$;
- $R(u, v) \ge 0$ if $u \ge u^*$, so in particular when $u \ge 1$.

To prove that v is not negative it is sufficient to take $\theta = v^-(t) = \frac{1}{2}(v(t) - |v(t)|)$ as test function in (11) to get

$$\|v^-(t)\|^2 \le \|v_0^-\|^2 + 2\int_0^t (R(u(\tau), v^-(\tau)), v^-(\tau))d\tau \le 0,$$

by which $v^-(t)$ is a zero element of $L^2(\Omega)$.

We now take $\omega = u^-(t)$ and $\psi = (u^-(t))^2$ in (11), and we exploit the non-negativity of v proven above and the properties of $R(u, v)$ to get, after integration by parts of the divergence term,

$$\frac{1}{2}\frac{d}{dt}\|u^-(t)\|^2 + \|\nabla u^-(t)\|^2 + \frac{1}{2}(\partial_t v, u^-(t)^2) \in -(R(u^-, v), u^-(t)) \le 0,$$

by which, since $\|u_0^-\| = 0$,

$$\|u^-(t)\|^2 + 2\int_0^t \|\nabla u^-(\tau)\|^2 d\tau \le \|u_0^-\|^2 + \frac{1}{2}\int_0^t (R(u^-(\tau), v(\tau)), u^-(\tau)^2)d\tau$$
$$\le \frac{1}{2}\int_0^t \|u^-(\tau)\|^2 d\tau.$$

By Gronwall's inequality we get $\|u^-(t)\| = 0$. The fact that u cannot exceed 1 is obtained in a similar way, by looking at the negative part of $1 - u$. Using these bounds for u we may prove that $v \le 1$ by looking at the negative part of $1 - v$. Note that $0 \le v(t) < 1$ and $0 \le u(t) \le 1$ for each $\epsilon > 0$, uniformly in ϵ.

Remark 6. Since the reaction rate $R(u,v)$ is zero (for $v=0$) or negative (for $v\neq 0$) for $0\leq u\leq 1$, v can only decrease from $v_0<1$ to zero, so that $v<1$ at all times. This is a consequence of the fact that only dissolution is considered, as expressed in Remark 2. Moreover, since $0\leq v(t)<1$ and $0\leq u(t)\leq 1$ independently of ϵ, there exists a constant $\epsilon_1>0$ such that, for each $0\leq\epsilon<\epsilon_1$, we have that

$$k_\epsilon(v):=\ k(\min\{1-\epsilon,v\})\equiv k(v).$$

Hence we obtain, by using a maximum principle argument, that the regularized Problem P_2 is equivalent to the unregularized problem.

By the definition of $k_\epsilon(v)$ we obtain that $\mu/k_\epsilon(v(t))\in L^\infty(\Omega)$ and is positive.
For what concerns the regularity of the solutions, we take $\omega=u(t)$ in (11), to obtain

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|u(t)\|^2+\|\nabla u(t)\|^2 &\in -\frac{1}{2}\Big(\partial_t v(t),u^2\Big)-\Big(\partial_t v(t),u\Big)\\ &=-\frac{1}{2}\Big(r(u)-H(v),u^2\Big)-\Big(r(u)-H(v),u\Big),\end{aligned}$$

after integrating by parts and using $(11)_2$ with $\psi=u^2$.
Since $r(u)$ is non-negative and $H(v)$ takes values between 0 and 1, the application of Cauchy–Schwarz and Young inequalities gives

$$\frac{1}{2}\frac{d}{dt}\|u(t)\|^2+\|\nabla u(t)\|^2\leq\frac{1}{2}\|u(t)\|^2+|\Omega|^{1/2}\|u(t)\|\leq\frac{|\Omega|}{2}+\|u(t)\|^2.$$

Then, thanks to Gronwall's inequality,

$$\|u(t)\|^2+2\int_0^t\|\nabla u(s)\|^2ds\leq(\|u_0\|^2+T|\Omega|)(1+Te^{2T})\quad\text{for } t\in(0,T]. \tag{12}$$

As for v, we take $\theta=v$ in (11); we use the local Lipschitz continuity of $r(u)$ and (12) to obtain that $\|v(t)\|$ is bounded uniformly in $(0,T]$.
The boundedness of $\partial_t v$, and consequently that of div $\mathbf{q}$, derives from that of $r(u)-H(v)$. If we choose $\boldsymbol{\tau}=\nabla\eta$ in (11), where η satisfies

$$\begin{cases}-\Delta\eta=p,\\ \eta|_{\Gamma_D}=0,\quad \frac{\partial\eta}{\partial n}=0 \text{ on } \Gamma_N,\end{cases}$$

we obtain $\|p\|^2\leq C+D_\epsilon\|\mathbf{q}\|^2$, thanks to the boundedness of $\mu/k_\epsilon(v)$ and to the Lax–Milgram estimate $\|\nabla\eta\|\leq C\|p\|$. The notation D_ϵ means that the value of the positive constant D_ϵ depends on ϵ.
We now take $\boldsymbol{\tau}=\mathbf{q}$ and $\psi=p$ in (11), exploit the facts that $0\leq H(v)\leq 1$, $r(u)$ is bounded and $k_\epsilon(v)$ is positively bounded away from zero, and use the estimate for $\|p\|$, to obtain $\|\mathbf{q}\|\leq C_\epsilon$.
Since $u\in L^2(0,T;H_0^1(\Omega))$ and $\mathbf{q}u\in L^\infty(0,T;L^2(\Omega))$, we have that $\partial_t u\in L^2(0,T;H^{-1}(\Omega))$. Note that, if $u_0\in H_0^1(\Omega)$, since $\mathbf{q}\in[L^\infty(\Omega)]^2$, by choosing $\omega=\partial_t u$, we obtain that $u\in L^\infty(0,T;H_0^1(\Omega))\cap H^1(0,T;L^2(\Omega))$. □

We are now in the position to prove Theorem 3:

Proof of Theorem 3. Assume there exist two solutions of (11), indicated by $(u_1,v_1,\mathbf{q}_1,p_1)$ and $(u_2,v_2,\mathbf{q}_2,p_2)$, and define: $\bar{u}=u_1-u_2$, $\bar{v}=v_1-v_2$, $\bar{\mathbf{q}}=\mathbf{q}_1-\mathbf{q}_2$, $\bar{p}=p_1-p_2$. We have at $t=0$ that $\bar{u}(0)=0$, $\bar{v}(0)=0$,

$\bar{\mathbf{q}}(0) = \mathbf{0}$ and $\bar{p}(0) = 0$. Taking $\theta = \bar{v}(t, \mathbf{x})$ from the fourth equation of system (11) we obtain

$$\frac{1}{2}\frac{d}{dt}\|\bar{v}\|^2 \in (r(u_1) - r(u_2), \bar{v}) - (H(v_1) - H(v_2), \bar{v}).$$

Using the monotonicity property of the set valued map $H(v)$ (note that this property is still valid with the prescription (4)), the Lipschitz continuity of $r(u)$ (with constant L_r) and Schwarz and Young inequalities, we obtain

$$\frac{d}{dt}\|\bar{v}(t,\mathbf{x})\|^2 \leq L_r^2\|\bar{u}(t,\mathbf{x})\|^2 + \|\bar{v}(t,\mathbf{x})\|^2.$$

We then have

$$\|\bar{v}(t,\mathbf{x})\|^2 \leq C\, e^T \int_0^t \|\bar{u}(s,\mathbf{x})\|^2 ds. \tag{13}$$

Taking now $\omega = \bar{u}(t, \mathbf{x})$ in the difference between equations $(11)_3$ for $(u_1, v_1, \mathbf{q}_1, p_1)$ and $(u_2, v_2, \mathbf{q}_2, p_2)$ we have

$$(\partial_t\bar{u}(t), \bar{u}(t)) + \|\nabla\bar{u}(t)\|^2 - (\bar{\mathbf{q}}u_1(t), \nabla\bar{u}(t)) - (\mathbf{q}_2\bar{u}(t), \nabla\bar{u}(t)) \in (\partial_t\bar{v}(t), \bar{u}(t)), \tag{14}$$

which we rewrite, after integration by parts of the fourth term and integration in time from 0 to $t < T$, as the following differential inclusion:

$$\frac{1}{2}\|\bar{u}(t)\|^2 + \int_0^t \|\nabla\bar{u}(s)\|^2 ds \in \int_0^t (\bar{\mathbf{q}}u_1(s), \nabla\bar{u}(s))ds - \frac{1}{2}\int_0^t \Big(\frac{\partial v_2(s)}{\partial t}, \bar{u}^2(s)\Big)ds$$
$$+ \int_0^t (H(v_1(s)) - H(v_2(s)), \bar{u}(s))ds - \int_0^t (r(u_1(s)) - r(u_2(s)), \bar{u}(t)). \tag{15}$$

We now introduce the following lemma.

Lemma 3. *Given two solutions of* (11), *indicated by* $(u_1, v_1, \mathbf{q}_1, p_1)$ *and* $(u_2, v_2, \mathbf{q}_2, p_2)$, *and defining:* $\bar{u} = u_1 - u_2$, $\bar{v} = v_1 - v_2$, *we have*

$$\|H(v_1) - H(v_2)\| \leq C\|\bar{u}\| + D\|\bar{v}\|. \tag{16}$$

Proof. Indeed, if $v_1 = v_2 = 0$, from (4), Lemma 2 and from the Lipschitz continuity of $r(u)$, we get the estimate $\|H(v_1) - H(v_2)\| \leq C\|\bar{u}\|$; if $v_1, v_2 \neq 0$, we get the estimate $\|H(v_1) - H(v_2)\| \leq D\|\bar{v}\|$; if $v_1 \neq 0$ and $v_2 = 0$ (or vice versa), from estimate (13) we have that $u_1 \neq u_2$ (almost everywhere in Ω), and from (4) we have $\|H(v_1) - H(v_2)\| \leq C\|1 - u_2\| \leq C\|\bar{u}\|$. □

Thanks to Lemma 2, the monotonicity and the Lipschitz continuity of $r(u)$, we can then write the following inequality:

$$\|\bar{u}(t)\|^2 + \int_0^t \|\nabla\bar{u}(s)\|^2 ds \leq C\int_0^t \|\bar{\mathbf{q}}(s)\|^2 ds + D\int_0^t \|\bar{u}(s)\|^2 ds + E\int_0^t \Big(\int_0^s \|\bar{u}(r)\|^2 dr\Big)ds,$$

which implies (see for instance [18])

$$\|\bar{u}(t)\|^2 \leq C\int_0^t \|\bar{\mathbf{q}}(\mathbf{s})\|^2 ds. \tag{17}$$

Taking the difference between the first and second equations of system (11) for $(u_2,\, v_2,\, \mathbf{q}_2,\, p_2)$ and $(u_1,\, v_1,\, \mathbf{q}_1,\, p_1)$, we obtain

$$\begin{cases} \left(\left[\frac{\mu}{k_\epsilon(v_1)} - \frac{\mu}{k_\epsilon(v_2)}\right]\mathbf{q_1}, \boldsymbol{\tau}\right) + \left(\frac{\mu}{k_\epsilon(v_2)}\bar{\mathbf{q}}, \boldsymbol{\tau}\right) - (\bar{p}, \operatorname{div}\boldsymbol{\tau}) = 0, \\ (\operatorname{div}\bar{\mathbf{q}}, \psi) = (\partial_t \bar{v}, \psi). \end{cases} \tag{18}$$

If we choose $\boldsymbol{\tau} = \nabla\eta$, where η satisfies

$$\begin{cases} -\Delta\eta = \bar{p}, \\ \eta|_{\Gamma_D} = 0, \quad \frac{\partial\eta}{\partial n} = 0 \text{ on } \Gamma_N, \end{cases}$$

the first equation of (18) provides

$$\|\bar{p}\|^2 + \left(\left[\frac{\mu}{k_\epsilon(v_1)} - \frac{\mu}{k_\epsilon(v_2)}\right]\mathbf{q_1}, \nabla\eta\right) + \left(\frac{\mu}{k_\epsilon(v_2)}\bar{\mathbf{q}}, \nabla\eta\right) = 0,$$

by which, thanks to Lemma 2, the Lax–Milgram estimate $\|\nabla\eta\| \leq \|\bar{p}\|$, the Lipschitz continuity property of $k_\epsilon(v)$ and (13), we finally obtain

$$\|\bar{p}\|^2 \leq C\|\bar{\mathbf{q}}\|\,\|\bar{p}\| + D\|\bar{p}\|\,\|\bar{v}\| \to \|\bar{p}\|^2 \leq C\|\bar{\mathbf{q}}\|^2 + D\int_0^t \|\bar{u}(s)\|^2 ds. \tag{19}$$

We now take $\boldsymbol{\tau} = \bar{\mathbf{q}}$ and $\psi = \bar{q}$ in (18), obtaining

$$\left(\left[\frac{\mu}{k_\epsilon(v_1)} - \frac{\mu}{k_\epsilon(v_2)}\right]\mathbf{q_1}, \bar{\mathbf{q}}\right) + \left(\frac{\mu}{k_\epsilon(v_2)}\bar{\mathbf{q}}, \bar{\mathbf{q}}\right) \in \big(r(u_1) - r(u_2), \bar{p}\big) - \big(H(v_1) - H(v_2), \bar{p}\big). \tag{20}$$

Since $r(u)$ and $k_\epsilon(v)$ are Lipschitz continuous, $\mathbf{q}$ is bounded, $1/k_\epsilon(v)$ is positively bounded away from zero, and given (16), we have that

$$\|\bar{\mathbf{q}}\|^2 \leq C\|\bar{u}\|\,\|\bar{p}\| + D\|\bar{v}\|\,\|\bar{p}\| + E\|\bar{v}\|\,\|\bar{\mathbf{q}}\|. \tag{21}$$

Combined with (19), it allows us to obtain

$$\|\bar{\mathbf{q}}\|^2 \leq C\|\bar{u}\|^2 + D\int_0^t \|\bar{u}(s)\|^2 ds, \tag{22}$$

which, substituted in (17), provides

$$\|\bar{u}(t)\|^2 \leq C\int_0^t \|\bar{u}(s)\|^2 ds + D\int_0^t \Big(\int_0^s \|\bar{u}(r)\|^2 dr\Big) ds, \tag{23}$$

and, consequently, $\|\bar{u}(t)\|^2 = 0$ [18]. As a consequence of (13), (22) and (19), we then have: $\|\bar{v}(t)\| = \|\bar{\mathbf{q}}(\mathbf{t})\| = \|\bar{p}(t)\| = 0$. □

2.5. Existence of solutions of the coupled problem

The existence of solutions is proved through a Faedo–Galerkin approach using a discretized problem. We write a discrete approximation of Problem P_2 by a finite difference scheme in time, a dual mixed hybridized finite element discretization in space for the Darcy equation and a primal hybrid finite element discretization in space for the species transport equations. Since for the numerical solution of the discrete ODE DRH we use event-driven methods [8] that employ the Filippov prescriptions, we have chosen an explicit Euler time discretization. The Euler semi-implicit method used in [14] (in the case of a given velocity field) is not feasible in our case, since it updates the v variable at a given time step using a value of the u variable at the next time step, which makes event-driven techniques impracticable.

Let $\mathcal{T}_h$ be a regular conforming decomposition of Ω into triangles, and let us introduce the following finite element spaces:

$$\mathcal{Z}_h := \{\mathbf{q}_h \in \prod_{K\in\mathcal{T}_h} \boldsymbol{H}_{\mathrm{div}}(K) | \mathbf{q}_{h|K} \in \mathbb{RT}_0(K)\ \forall K \in \mathcal{T}_h\},$$

$$\mathcal{V}_h := \{p_h \in L^2(\Omega) | p_{h|K} \in \mathbb{P}_0(K)\ \forall K \in \mathcal{T}_h\},$$

$$\mathcal{P}_h := \{\lambda_h \in \prod_{K\in\mathcal{T}_h} H^{1/2}(\partial K) | \lambda_{h|\partial K} \in \mathbb{P}_0(\partial K)\ \forall K \in \mathcal{T}_h, \lambda_{h|\partial\Omega} = 0\},$$

$$\mathcal{W}_h := \{v_h \in \prod_{K\in\mathcal{T}_h} H^1(K) | v_{h|K} \in \mathbb{P}_1(K)\ \forall K \in \mathcal{T}_h\},$$

$$\mathcal{Q}_h := \{\mu_h \in \prod_{K\in\mathcal{T}_h} H^{-1/2}(\partial K) | \mu_{h|\partial K} \in \mathbb{P}_0(\partial K)\ \forall K \in \mathcal{T}_h\},$$

where $\mathbb{P}_i(K)$ indicates the space of polynomials of order i on K, $\mathbb{RT}_0(K)$ is the zero-th order Raviart–Thomas space, and $\mathbb{P}_0(\partial K)$ is the zero-th order polynomial on each edge of ∂K. Introducing the local projection operators $\Pi_K : \boldsymbol{H}_{\mathrm{div}}(K) \to \mathbb{RT}_0(K)$; $P^0_K : L^2(K) \to \mathbb{P}_0(K)$; $P^1_K : H^1(K) \to \mathbb{P}_1(K)$; $\rho_K : \prod_{K\in\mathcal{T}_h} L^2(\partial K) \to \mathbb{R}_0(\partial K)$, we recall some well known results from interpolation theory [5].

$$\begin{aligned}
&\|\boldsymbol{\tau} - \Pi_K\boldsymbol{\tau}\|_{0,K} \le C h_K \|\boldsymbol{\tau}\|_{1,K}, \quad \text{for} \quad \boldsymbol{\tau} \in \left[H^1(K)\right]^2,\\
&\|\operatorname{div}(\boldsymbol{\tau} - \Pi_K\boldsymbol{\tau})\|_{0,K} \le C h_K \|\operatorname{div}\boldsymbol{\tau}\|_{1,K}, \quad \text{for} \quad \operatorname{div}\boldsymbol{\tau} \in H^1(K),\\
&\|v - P^0_K v\|_{0,K} \le C h_K \|v\|_{1,K}, \quad \text{for} \quad v \in H^1(K),\\
&\|v - P^1_K v\|_{0,K} \le C h_K \|v\|_{1,K}, \quad \text{for} \quad v \in H^1(K),\\
&\|\lambda - \rho_K\lambda\|_{1/2,e_h} \le C h_K \|w\|_{2,K}, \quad \text{for} \quad w \in H^2(K) | w_{|\partial K} = \lambda,\\
&\|\lambda - \rho_K\lambda\|_{-1/2,e_h} \le C h_K \|\operatorname{div}\mathbf{q}\|_{1,K}, \quad \text{for} \quad \mathbf{q} \in \left[H^2(K)\right]^2 \mid \mathbf{q}\cdot\mathbf{n}_{|\partial K} = \lambda,
\end{aligned} \tag{24}$$

where e_h is the set of edges of K. We set $\tau = T/N$ for an $N \in \mathbb{N}$, and $t_n = n\tau$, $n = 1, \ldots, N$. Starting with $u^0_h = P_h u_0$ and $v^0_h = P_h v_0$, where P_h is a global interpolation operator, with $u_0 \in H^1_0(\Omega)$ and $v_0 \in L^2(\Omega)$, we define

Problem $\mathbf{P}^{h}_{2}$. Given $(u^{n-1}_h, v^{n-1}_h) \in \mathcal{U}_h \times \mathcal{U}_h$, find $(\mathbf{q}^n_h, p^n_h, \lambda^n_h) \in \mathcal{Z}_h \times \mathcal{V}_h \times \mathcal{P}_h$ and $(u^n_h, v^n_h, \mu^n_h) \in \mathcal{W}_h \times \mathcal{W}_h \times \mathcal{Q}_h$, such that for all $(\boldsymbol{\tau}_h, \psi_h, \rho_h) \in \mathcal{Z}_h \times \mathcal{V}_h \times \mathcal{P}_h$ and $(\omega_h, \theta_h, \nu_h) \in \mathcal{W}_h \times \mathcal{W}_h \times \mathcal{Q}_h$,

$$
\begin{cases}
\sum_{K\in\mathcal{T}_h}\Big[\int\limits_K \frac{\mu}{k_\epsilon(v_h^{n-1})}\mathbf{q}_h^n\cdot\boldsymbol{\tau}_h - \int\limits_K p_h^n \operatorname{div}\boldsymbol{\tau}_h + \int\limits_{\partial K}\lambda_h^n\boldsymbol{\tau}_h\cdot\mathbf{n} + \int\limits_{\partial K\cap\Gamma_D} p_D\boldsymbol{\tau}_h\cdot\mathbf{n}\Big] = 0,\\
\sum_{K\in\mathcal{T}_h}\Big[\int\limits_K \psi_h \operatorname{div}\mathbf{q}_h^n\Big] = \int\limits_\Omega \big(r(u_h^{n-1}) - H(v_h^{n-1})\big)\psi_h,\\
\sum_{K\in\mathcal{T}_h}\int\limits_{\partial K}\rho_h\mathbf{q}_h^n\cdot\mathbf{n} = 0,\\
\sum_{K\in\mathcal{T}_h}\Big[\int\limits_K (u_h^n - u_h^{n-1})\omega_h + \tau\int\limits_K \nabla u_h^n\nabla\omega_h - \tau\int\limits_K \mathbf{q}_h^n u_h^n\nabla\omega_h - \tau\int\limits_{\partial K}\mu_h^n\omega_h\Big]\\
\quad = -\tau\int\limits_\Omega (r(u_h^{n-1}) - H(v_h^{n-1}))\omega_h,\\
\int\limits_\Omega (v_h^n - v_h^{n-1})\theta_h \in \tau\int\limits_\Omega (r(u_h^{n-1}) - H(v_h^{n-1}))\theta_h,\\
\sum_{K\in\mathcal{T}_h}\int\limits_{\partial K} u_h^n\nu_h = 0.
\end{cases}
\tag{25}
$$

This particular choice of finite elements is useful for the analysis, since we can easily treat the terms element-wise. However, we wish to point out that numerical experiments show the suitability of more standard finite element discretizations.

Defining the operator $B := (B\mathbf{q}\cdot\mathbf{n},\rho) = \sum_K \int_{\partial K}\rho\mathbf{q}\cdot\mathbf{n}\ \forall\rho\in\prod_{K\in\mathcal{T}_h}H^{1/2}(\partial K), \rho_{\partial\Omega} = 0$, we can identify $\boldsymbol{H}_{\mathrm{div}}(\Omega) = \ker B$. Having introduced a finite element space $\mathcal{P}_h$ of functions in $\mathbb{P}_0(\partial K)$, which are discontinuous at the edge vertices of ∂K, the formulation enforces the local reciprocity constraint [5].

Analogously, by defining the operator $C := (Cv,\mu) = \sum_K \int_K v\mu\ \forall\mu\in\prod_{K\in\mathcal{T}_h}H^{-1/2}(\partial K)$ we can identify $H_0^1(\Omega) = \ker C$. Since $\mathcal{Q}_{h|K} = \mathbb{P}_0(\partial K)$, the space $\ker C_h$ is given by functions in $\mathcal{W}_h$ which are continuous at the middle point of each edge of ∂K; the formulation is thus equivalent to a non-conforming primal formulation on a Crouzier–Raviart finite element space [5].

Remark 7. Note that we cannot exploit a maximum principle, since, for our kind of problem and for the finite element spaces we are using, there are no standard discrete maximum principles. Hence, we cannot show that if $u_h^{n-1}\le 1$ then $u_h^n\le 1$ for a sufficiently small time step, nor that $v_h^n<1$ if $v_h^{n-1}<1$. However, the introduction of the regularization of permeability $k_\epsilon(v_h)$ avoids the problem of low regularity of the Darcy field due to the degeneracy at $v_h = 1$. Moreover, discrete maximum principle which guarantees that if $u_h^{n-1}\le 1$ then $u_h^n\le 1$ is available in the case $v_{h|K}\in\mathbb{P}_0(K)$.

The possibility of negative concentrations of v_h^n and u_h^n, which can be obtained when $v_h^{n-1}\ll 1$, $v_h^{n-1}\neq 0$, $r(u_h^{n-1})\ll 1$ and the time step τ is greater than a given $\tau^*\ll 1$, can be avoided by localizing the threshold $v = 0$ with an event driven strategy, like the ones in [7,8].

From the fourth and fifth equations of system (11), by applying elliptic regularity on each element K and noting that the forcing term $r(u_h^{n-1}) - H(v_h^{n-1})\in L^2(K)$, we obtain that $u_h, v_h\in L^\infty(K)$, and $k_\epsilon(v_h)\in L^\infty(K)$.

Existence and uniqueness of the solution to Problem P_2^h derive from the following facts:

- The term $\mu/k_\epsilon(v_h^{n-1})$ is bounded and always positive, the quadratic form $(\frac{\mu}{k_\epsilon(v_h^{n-1})}\mathbf{q}_h^n,\mathbf{q}_h^n)_K$ is continuous and coercive over $\ker B_h$, the finite dimensional spaces satisfy the discrete inf–sup condition and the forcing terms are well defined. Therefore the mixed hybridized formulation of the Darcy equations has a unique solution [5].
- The bilinear form associated to the transport equation for u_h is weakly coercive over $\ker C_h$, the finite dimensional spaces satisfy the discrete inf–sup condition and the forcing term is well defined. Therefore, the primal hybrid formulation for u_h^n has a unique solution [5].

- The application of the Filippov selection procedure ensures that there exists a unique sequence of solutions v_h^n, which converges, for $N \to \infty$, to the unique solution of the continuous in time inclusion problem uniformly in $C^0([0,T],\mathbb{R}^2)$ [9].

We proceed now to obtain energy estimates, which will be used later to show the convergence of a time continuous approximation of the discrete solutions to the weak solution of the continuous problem. To ease notation, from now on, where not otherwise indicated, the sum over all the elements K of the mesh is understood.

Lemma 4 *(Energy estimates). There exist constants $C > 0$ independent of τ and h such that the following estimates hold:*

$$\sup_{k=1,\dots,N} \|v_h^k - v_h^{k-1}\|_K + \sum_{n=1}^{N} \|u_h^n - u_h^{n-1}\|_K^2 \leq C\tau, \tag{26}$$

$$\sum_{n=1}^{N} \|\nabla(u_h^n - u_h^{n-1})\|_K^2 + \tau \sum_{n=1}^{N} \|\nabla u_h^n\|_K^2 \leq C, \tag{27}$$

$$\sup_{k=1,\dots,N} \|\mathbf{q}_h^k\|_K \leq C, \tag{28}$$

$$\sup_{k=1,\dots,N} \|p_h^k\|_K + \sup_{k=1,\dots,N} \|\lambda_h^k\|_{\partial K} \leq C, \tag{29}$$

$$\sum_{n=1}^{N} \|\mathbf{q}_h^n - \mathbf{q}_h^{n-1}\|_K^2 \leq C\tau, \tag{30}$$

$$\sum_{n=1}^{N} \|p_h^n - p_h^{n-1}\|_K^2 + \sum_{n=1}^{N} \|\lambda_h^n - \lambda_h^{n-1}\|_{\partial K}^2 \leq C\tau, \tag{31}$$

$$\tau \sum_{n=1}^{N} \|\operatorname{div} \mathbf{q}_h^n\|_K^2 \leq C, \tag{32}$$

$$\sum_{n=1}^{N} \|\operatorname{div}(\mathbf{q}_h^n - \mathbf{q}_h^{n-1})\|_K^2 \leq C\tau. \tag{33}$$

Proof. We take $\omega_h = u_h^n$ and $\nu_h = \mu_h^n$ in the fourth and in the sixth equations of system (25), respectively, to have

$$\frac{1}{2}\left[\|u_h^n\|_K^2 - \|u_h^{n-1}\|_K^2 + \|u_h^n - u_h^{n-1}\|_K^2\right] + \tau\|\nabla u_h^n\|_K^2 + \tau(r(u_h^{n-1}) - H(v_h^{n-1}), (u_h^n)^2)_K$$
$$= -\tau(r(u_h^{n-1}) - H(v_h^{n-1}), u_h^n)_K.$$

Since $r(\cdot)$ is positive, the term $(r(u_h^{n-1}), (u_h^n)^2)$ is positive. Using the boundedness of $H(\cdot)$, the Lipschitz continuity of $r(\cdot)$, Cauchy–Schwarz and Young inequalities, we obtain

$$\frac{1}{2}\left(\|u_h^n\|_K^2 - \|u_h^{n-1}\|_K^2 + \|u_h^n - u_h^{n-1}\|_K^2\right) + \tau\|\nabla u_h^n\|_K^2$$
$$\leq C\tau\|u_h^n\|_K^2 + \tau L_r\|u_h^{n-1}\|_K\|u_h^n\|_K + C\tau\|u_h^n\|_K \leq C\tau\|u_h^n\|_K^2 + C\tau\|u_h^{n-1}\|_K^2 + C\tau + \frac{1}{2}\tau\|u_h^n\|_K^2,$$

and, by summing over $n = 1, \dots, k$, for an arbitrary $k \leq N$,

$$\frac{1}{2}\|u_h^k\|_K^2 + \frac{1}{2}\sum_{n=1}^{k} \|u_h^n - u_h^{n-1}\|_K^2 + \tau\sum_{n=1}^{k} \|\nabla u_h^n\|_K^2 \leq \frac{1}{2}\|u_h^I\|_K^2 + C.$$

Here we have used the fact that $u_h^n \in L^\infty(K) \subset L^2(K)$. This result implies the estimate in the second part of (27).

Remark 8. The same result could be obtained by using the discrete Gronwall inequality, in this case we do not need $u_h^n \in L^\infty(K)$. Moreover, we could obtain the same result without taking an integration by parts of the advection term in the fourth equation of system (25), by using the fact that $\mathbf{q}_h^n \in [L^\infty(K)]^2$, or the estimate of $\|\mathbf{q}_h^n\|$ given by (35), and applying the discrete Gronwall inequality.

We take now $\theta_h = v_h^n - v_h^{n-1}$ in the fifth equation of system (25), consequently the first part of (26) gives

$$\|v_h^n - v_h^{n-1}\|_K^2 \leq \tau\|r(1)\|_K\,\|v_h^n - v_h^{n-1}\|_K + \tau C\|v_h^n - v_h^{n-1}\|_K.$$

To obtain (28) and (29), we take $\boldsymbol{\tau}_h = \Pi_K \nabla \eta_h$ in the first equation of system (25), where η_h is a solution of

$$\begin{cases} -\operatorname{div}\nabla\eta_h = p_h^n & \text{in} \quad K, \\ \nabla\eta_h \cdot \mathbf{n}|_{\partial K} = \lambda_h^n. \end{cases} \tag{34}$$

Note that $\operatorname{div}[\Pi_K\nabla\eta_h] = P_{k,0}\operatorname{div}\nabla\eta_h = -P_{k,0}p_h^n = -p_h^n$, and that $\Pi_K\nabla\eta_h \in \mathbb{RT}_0(K)$. Besides, for each K, $\|\Pi_K\nabla\eta_h\|_K \leq Ch\|p_h^n\|_K$. Then

$$\begin{aligned} \|p_h^n\|_K^2 + \|\lambda_h^n\|_{\partial K}^2 &= -(p_D, \lambda_h^n)_{\partial K\cap\Gamma_D} - \left(\frac{\mu}{k_\epsilon(v_h^{n-1})}\mathbf{q}_h^n, \Pi_K\nabla\eta_h\right)_K \\ &= -(\tilde{p}_D, p_h^n)_K - (\nabla\tilde{p}_D, \Pi_K\nabla\eta_h)_K - \left(\frac{\mu}{k_\epsilon(v_h^{n-1})}\mathbf{q}_h^n, \Pi_K\nabla\eta_h\right)_K \\ &\leq \frac{1}{4}\|p_h^n\|_K^2 + C + C\sup_K\left[\frac{\mu}{k_\epsilon(v_h^{n-1})}\right]\|\mathbf{q}_h^n\|_K\,\|p_h^n\|_K \leq \frac{1}{2}\|p_h^n\|_K^2 + C + C\|\mathbf{q}_h^n\|_K^2, \end{aligned}$$

where $\tilde{p}_D$ is a harmonic lifting of the boundary data. Hence, we may write

$$\|p_h^n\|_K^2 + \|\lambda_h^n\|_{\partial K}^2 \leq C(1 + \|\mathbf{q}_h^n\|_K^2).$$

Now, let us take $\boldsymbol{\tau}_h = \mathbf{q}_h^n$, $\psi_h = p_h^n$ and $\rho_h = \lambda_h^n$ in the first, the second and the third equations of system (25), respectively. We obtain

$$\left(\frac{\mu}{k_\epsilon(v_h^{n-1})}\mathbf{q}_h^n, \mathbf{q}_h^n\right)_K - (r(u_h^{n-1}) - H(v_h^{n-1}), p_h^n)_K = -(\tilde{p}_D, r(u_h^{n-1}) - H(v_h^{n-1}))_K - (\nabla\tilde{p}_D, \mathbf{q}_h^n)_K. \tag{35}$$

Since $1/k_\epsilon$ is positive and bounded away from zero, we can write

$$\|\mathbf{q}_h^n\|_K^2 \leq \frac{1}{4C_p}\|p_h^n\|_K^2 + C + \frac{1}{4}\|\mathbf{q}_h^n\|_K^2 \leq \frac{1}{2}\|\mathbf{q}_h^n\|_K^2 + C,$$

where C_p is the constant C in the inequality $\|p_h^n\|_K^2 \leq D + C\|\mathbf{q}_h^n\|^2$. We thus obtain estimates (28) and (29).

If we take now $\psi_h = \operatorname{div}\mathbf{q}_h^n$ in the second equation of system (25), we get

$$\tau\|\operatorname{div}\mathbf{q}_h^n\|_K^2 \leq \tau\|r(u_h^{n-1}) - H(v_h^{n-1})\|_K\|\operatorname{div}\mathbf{q}_h^n\|_K \leq C\tau + \frac{1}{2}\tau\|\operatorname{div}\mathbf{q}_h^n\|_K^2,$$

and, by summing over $n = 1, \ldots, k$, for a $k \leq N$, we are able to obtain (32).

Taking $\omega_h = u_h^n - u_h^{n-1}$ and $\nu_h = \mu_h^n$ in the fourth and in the sixth equations of system (25), respectively, allows us to write that

$$\|u_h^n - u_h^{n-1}\|_K^2 + \tau(\nabla u_h^n, \nabla(u_h^n - u_h^{n-1}))_K - \tau(\mathbf{q}_h^n u_h^n, \nabla(u_h^n - u_h^{n-1}))_K = -(v_h^n - v_h^{n-1}, u_h^n - u_h^{n-1})_K.$$

Then, by applying integration by parts to the term $(\mathbf{q}_h^n u_h^n, \nabla(u_h^n - u_h^{n-1}))_K$, using the Cauchy and Young inequalities, equations (26), (28) and (32) and the fact that $\nabla u_h^n \in L^\infty(K)$ (since $u_h^n \in L^\infty(K) \cap \mathbb{P}_1(K)$), we get

$$\begin{aligned}
&\|u_h^n - u_h^{n-1}\|_K^2 + \frac{1}{2}\tau\big(\|\nabla u_h^n\|_K^2 - \|\nabla u_h^{n-1}\|_K^2 + \|\nabla(u_h^n - u_h^{n-1})\|_K^2\big)\\
&\quad = -\tau(u_h^n \operatorname{div} \mathbf{q}_h^n, (u_h^n - u_h^{n-1}))_K - \tau(\mathbf{q}_h^n \nabla u_h^n, (u_h^n - u_h^{n-1}))_K - (v_h^n - v_h^{n-1}, u_h^n - u_h^{n-1})_K\\
&\quad \le C\tau^2 + \frac{1}{6}\|u_h^n - u_h^{n-1}\|_K^2 + C\tau^2 + \frac{1}{6}\|u_h^n - u_h^{n-1}\|_K^2 + C\tau^2 + \frac{1}{6}\|u_h^n - u_h^{n-1}\|_K^2,
\end{aligned}$$

by which we can write

$$\frac{1}{2}\sum_{n=1}^{k}\|u_h^n - u_h^{n-1}\|_K^2 + \frac{1}{2}\tau\|\nabla u_h^k\|_K^2 + \frac{1}{2}\tau\sum_{n=1}^{k}\|\nabla u_h^n - \nabla u_h^{n-1}\|_K^2 \le \|\nabla u_h^0\|^2\tau + C\tau,$$

and obtain the second part of (26), and the first part of (27).

We now set $\psi_h = \operatorname{div}[\mathbf{q}_h^n - \mathbf{q}_h^{n-1}]$ and take the difference between the equations written at time n and $n-1$. Thanks to (16) and Young and Cauchy–Schwarz inequalities, we obtain

$$\begin{aligned}
\tau\|\operatorname{div}[\mathbf{q}_h^n - \mathbf{q}_h^{n-1}]\|_K^2 \le C\tau\|u_h^{n-1} - u_h^{n-2}\|_K^2 + \frac{1}{4}\tau\|\operatorname{div}[\mathbf{q}_h^n - \mathbf{q}_h^{n-1}]\|_K^2 + D\tau\|v_h^{n-1} - v_h^{n-2}\|_K^2\\
+ \frac{1}{4}\tau\|\operatorname{div}[\mathbf{q}_h^n - \mathbf{q}_h^{n-1}]\|_K^2. \qquad (36)
\end{aligned}$$

Estimate (33) is thus obtained by using (26), summing over $n = 1, \ldots, k$, for a $k \le N$, and setting $u_h^{-1} = u_h^0$, $v_h^{-1} = v_h^0$.

We proceed by taking $\boldsymbol{\tau}_h = \mathbf{q}_h^n - \mathbf{q}_h^{n-1}$ and $\rho_h = \lambda_h^n$ in the first and the third equations of system (25), respectively, and considering the difference between the equations written at times n and $(n-1)$, obtaining that

$$\begin{aligned}
&\tau\left(\frac{\mu}{k_\epsilon(v_h^{n-2})}[\mathbf{q}_h^n - \mathbf{q}_h^{n-1}], [\mathbf{q}_h^n - \mathbf{q}_h^{n-1}]\right)_K\\
&\quad = -\tau\left(\left[\frac{\mu}{k_\epsilon(v_h^{n-1})} - \frac{\mu}{k_\epsilon(v_h^{n-2})}\right]\mathbf{q}_h^n, [\mathbf{q}_h^n - \mathbf{q}_h^{n-1}]\right)_K + \tau(p_h^n - p_h^{n-1}, \operatorname{div}[\mathbf{q}_h^n - \mathbf{q}_h^{n-1}])_K. \qquad (37)
\end{aligned}$$

We estimate the first term on the right hand side using the fact that $\mathbf{q}_h^n \in [L^\infty(K)]^2$ and that the function $[k_\epsilon(v_h)]^{-1}$ is Lipschitz continuous. The application of Young inequality and (26) gives

$$\tau\left(\left[\frac{\mu}{k_\epsilon(v_h^{n-1})} - \frac{\mu}{k_\epsilon(v_h^{n-2})}\right]\mathbf{q}_h^n, [\mathbf{q}_h^n - \mathbf{q}_h^{n-1}]\right)_K \le \frac{1}{2}\tau\|\mathbf{q}_h^n - \mathbf{q}_h^{n-1}\|^2 + C\tau^3.$$

Hence, since $[k_\epsilon(v_h^{n-2})]^{-1}$ is positive and bounded away from zero, and thanks to (36), we get from (37) that

$$\frac{1}{2}\tau\|\mathbf{q}_h^n - \mathbf{q}_h^{n-1}\|_K^2 \le C\tau^3 + D\tau\|\operatorname{div}[\mathbf{q}_h^n - \mathbf{q}_h^{n-1}]\|_K\|p_h^n - p_h^{n-1}\|_K \le C\tau^3 + D\tau^2\|p_h^n - p_h^{n-1}\|_K.$$

Summing over $n = 1, \dots, k$, for a $k \le N$, it is now possible to show that

$$\tau \sum_{n=1}^{k} \|\mathbf{q}_h^n - \mathbf{q}_h^{n-1}\|_K^2 \le C\tau^2 + D\tau^2 \sum_{n=1}^{k} \|p_h^n - p_h^{n-1}\|_K. \tag{38}$$

Now, we set $\boldsymbol{\tau}_h = \Pi_K \nabla \eta_h$ in the first equation of system (25), where

$$\begin{cases} -\operatorname{div} \nabla \eta_h = p_h^n - p_h^{n-1} & \text{in} \quad K, \\ \nabla \eta_h \cdot \mathbf{n}|_{\partial K} = \lambda_h^n - \lambda_h^{n-1} \end{cases}$$

and take the difference between the equations written at times n and $(n-1)$, obtaining that

$$\begin{aligned} &\|p_h^n - p_h^{n-1}\|_K^2 + \|\lambda_h^n - \lambda_h^{n-1}\|_K^2 \\ &\quad = \left(\left[\frac{\mu}{k_\epsilon(v_h^{n-1})} - \frac{\mu}{k_\epsilon(v_h^{n-2})} \right] \mathbf{q}_h^n, \Pi_K \nabla \eta_h \right)_K + \left(\frac{\mu}{k_\epsilon(v_h^{n-2})} [\mathbf{q}_h^n - \mathbf{q}_h^{n-1}], \Pi_K \nabla \eta_h \right)_K. \end{aligned} \tag{39}$$

The first term in the right hand side can be bounded using a trilinear Hölder inequality (or using the fact that $\mathbf{q}_h^n \in [L^\infty(K)]^2$), noting that, at the discrete level, $\|\nabla \mathbf{q}_h^n\|_K = \|\operatorname{div} \mathbf{q}_h^n\|_K$, since $\mathbf{q}_h^n \in \mathbb{RT}_0(K)$. Hence

$$\begin{aligned} \left(\left[\frac{\mu}{k_\epsilon(v_h^{n-1})} - \frac{\mu}{k_\epsilon(v_h^{n-2})} \right] \mathbf{q}_h^n, \Pi_K \nabla \eta_h \right)_K &\le C\tau \|\Pi_K \nabla \eta_h\|_{[H^1(K)]^2} \|\mathbf{q}_h^n\|_{[H^1(K)]^2} \\ &\le \frac{1}{4} \|p_h^n - p_h^{n-1}\|_K^2 + C\tau^2 + D\tau^2 \|\operatorname{div} \mathbf{q}_h^n\|_K^2. \end{aligned}$$

The second term in the right hand side can be bounded using the Cauchy–Schwarz inequality and the boundedness of the permeability,

$$\left(\frac{\mu}{k_\epsilon(v_h^{n-2})} [\mathbf{q}_h^n - \mathbf{q}_h^{n-1}], \Pi_K \nabla \eta_h \right)_K \le \frac{1}{4} \|p_h^n - p_h^{n-1}\|_K^2 + C \|\mathbf{q}_h^n - \mathbf{q}_h^{n-1}\|_K^2. \tag{40}$$

Thanks to equation (32), we may write

$$\frac{1}{2} \sum_{n=1}^{k} \|p_h^n - p_h^{n-1}\|_K^2 + \sum_{n=1}^{k} \|\lambda_h^n - \lambda_h^{n-1}\|_{\partial K}^2 \le C\tau + D \sum_{n=1}^{k} \|\mathbf{q}_h^n - \mathbf{q}_h^{n-1}\|_K^2, \tag{41}$$

and, by substituting (38) into (41), we get

$$\sum_{n=1}^{k} \|p_h^n - p_h^{n-1}\|_K^2 \le C\tau + D\tau \sum_{n=1}^{k} \|p_h^n - p_h^{n-1}\|_K. \tag{42}$$

This inequality can be refined starting from the following identity:

$$\left(\sum_{n=1}^{k} \|p_h^n - p_h^{n-1}\|_K \right)^2 + \sum_{n=1}^{k} \sum_{m>n}^{k} ([\|p_h^n - p_h^{n-1}\|_K - \|p_h^m - p_h^{m-1}\|_K])^2 = k \sum_{n=1}^{k} \|p_h^n - p_h^{n-1}\|_K^2,$$

which, substituted into (42), gives

$$\left(\sum_{n=1}^{k} \|p_h^n - p_h^{n-1}\|_K \right)^2 \le \frac{C}{\tau} \sum_{n=1}^{k} \|p_h^n - p_h^{n-1}\|_K^2 \le C + D \sum_{n=1}^{k} \|p_h^n - p_h^{n-1}\|_K. \tag{43}$$

This quadratic inequality implies that

$$\sum_{n=1}^{k} \|p_h^n - p_h^{n-1}\|_K \leq C. \tag{44}$$

Using (44) in (38), we get estimate (30), while using (30) in (41), we get estimate (31). □

We now associate to the sequence of discrete solutions $(\mathbf{q}_h^n, p_h^n, \lambda_h^n, u_h^n, v_h^n)$ of Problem P_2^h the following time continuous approximation:

$$\begin{aligned}
&\mathbf{Q}_h^\tau(t) := \mathbf{q}_h^n \frac{t-t_{n-1}}{\tau} + \mathbf{q}_h^{n-1}\frac{t_n - t}{\tau}, \quad P_h^\tau(t) = p_h^n \frac{t-t_{n-1}}{\tau} + p_h^{n-1}\frac{t_n-t}{\tau},\\
&\Lambda_h^\tau(t) = \lambda_h^n \frac{t-t_{n-1}}{\tau} + \lambda_h^{n-1}\frac{t_n-t}{\tau},\\
&U_h^\tau(t) := u_h^n \frac{t-t_{n-1}}{\tau} + u_h^{n-1}\frac{t_n-t}{\tau}, \quad V_h^\tau(t) := v_h^n \frac{t-t_{n-1}}{\tau} + v_h^{n-1}\frac{t_n-t}{\tau},
\end{aligned} \tag{45}$$

for $t \in [t_{n-1}, t_n]$, $n = 1, \cdots, N$. They are a family of linear time interpolants that depend on the parameters h and τ.

To simplify the notation we introduce the following: $(f,g)_A^T = \int_0^T (f(t), g(t))_A dt$ for a given $L^2(A)$ product $(f,g)_A$, omitting A if $A = \Omega$. It effectively indicates the $L^2((0,T), L^2(A))$ product. While $(f,g)_A^{t_n} = \int_{t_{n-1}}^{t_n} (f(t), g(t))_A dt$ is used to indicate the $L^2((t_{n-1}, t_n), L^2(A))$ product.

We consider system (25), by multiplying it by a $C^1([0,T])$ function which is zero at T and integrating in time from 0 to T, to obtain that $(\mathbf{Q}_h^\tau, P_h^\tau, \Lambda_h^\tau, U_h^\tau, V_h^\tau)$ satisfies the following weak formulation:

For any $\boldsymbol{\tau} \in L^2((0,T); \prod_{K\in\mathcal{T}_h} \boldsymbol{H}_{\mathrm{div}}(K))$, $\psi \in L^2((0,T); \prod_{K\in\mathcal{T}_h} L^2(K))$, $\rho \in L^2((0,T); \prod_{K\in\mathcal{T}_h} H^{1/2}(\partial K))$, $\omega \in L^2((0,T); H_0^1(\Omega))$, $\theta \in L^2((0,T); L^2(\Omega))$, given $\boldsymbol{\tau}_h = \Pi_K \tau$, $\psi_h = P_{k,0}\psi$, $\rho_h = \rho_K \rho$, $\omega_h = P_{k,1}\omega$, $\theta_h = P_{k,1}\theta$,

$$\left\{\begin{aligned}
&(\tfrac{\mu}{k_\epsilon(V_h^\tau)}\mathbf{Q}_h^\tau, \boldsymbol{\tau})_K^T - (P_h^\tau, \operatorname{div}\boldsymbol{\tau})_K^T + (\Lambda_h^\tau, \boldsymbol{\tau}\cdot\mathbf{n})_{\partial K}^T + (p_D, \boldsymbol{\tau}\cdot\mathbf{n})_{\partial K\cap\Gamma_D}^T\\
&\quad = \textstyle\sum_{n=1}^N \Big[(\tfrac{\mu}{k_\epsilon(V_h^\tau)}\mathbf{Q}_h^\tau, [\boldsymbol{\tau} - \boldsymbol{\tau}_h])_K^{t_n} + ([\tfrac{\mu}{k_\epsilon(V_h^\tau)} - \tfrac{\mu}{k_\epsilon(v_h^n)}]\mathbf{Q}_h^\tau, \boldsymbol{\tau}_h)_K^{t_n} + (\tfrac{\mu}{k_\epsilon(V_h^\tau)}[\mathbf{Q}_h^\tau - \mathbf{q}_h^n], \boldsymbol{\tau}_h)_K^{t_n}\\
&\qquad - ([\tfrac{\mu}{k_\epsilon(V_h^\tau)} - \tfrac{\mu}{k_\epsilon(v_h^n)}][\mathbf{Q}_h^\tau - \mathbf{q}_h^n], \boldsymbol{\tau}_h)_K^{t_n} - (P_h^\tau, \operatorname{div}[\boldsymbol{\tau} - \boldsymbol{\tau}_h])_K^{t_n} - ([P_h^\tau - p_h^n], \operatorname{div}\boldsymbol{\tau}_h)_K^{t_n}\\
&\qquad + \textstyle\sum_{n=1}^N (\Lambda_h^\tau, [\boldsymbol{\tau}-\boldsymbol{\tau}_h]\cdot\mathbf{n})_{\partial K}^{t_n} + \sum_{n=1}^N ([\Lambda_h^\tau - \lambda_h^n], \boldsymbol{\tau}_h\cdot\mathbf{n})_{\partial K}^{t_n} + \sum_{n=1}^N (p_D, [\boldsymbol{\tau}-\boldsymbol{\tau}_h]\cdot\mathbf{n})_{\partial K\cap\Gamma_D}^{t_n}\Big],\\
&(\operatorname{div}\mathbf{Q}_h^\tau, \psi)_K^T - (\partial_t V_h^\tau, \psi)_K^T = \textstyle\sum_{n=1}^N \Big[(\operatorname{div}\mathbf{Q}_h^\tau, [\psi - \psi_h])_K^{t_n} + (\operatorname{div}[\mathbf{Q}_h^\tau - \mathbf{q}_h^n], \psi_h)_K^{t_n}\\
&\quad - (\partial_t V_h^\tau, [\psi - \psi_h])_K^{t_n}\Big],\\
&(\mathbf{Q}_h^\tau\cdot\mathbf{n}, \rho)_{\partial K}^T = \textstyle\sum_{n=1}^N \Big[(\mathbf{Q}_h^\tau\cdot\mathbf{n}, [\rho - \rho_h])_{\partial K}^{t_n} + \int_{t_{n-1}}^{t_n} ([\mathbf{Q}_h^\tau - \mathbf{q}_h^n]\cdot\mathbf{n}, \rho_h)_{\partial K}^{t_n}\Big],\\
&(\partial_t U_h^\tau, \omega)^T + (\nabla U_h^\tau, \nabla\omega)^T - (\mathbf{Q}_h^\tau U_h^\tau, \nabla\omega)^T + (\partial_t V_h^\tau, \omega)^T\\
&\quad = \textstyle\sum_{n=1}^N \Big[(\partial_t U_h^\tau, [\omega - \omega_h])^{t_n} + \int_{t_{n-1}}^{t_n} (\partial_t V_h^\tau, [\omega-\omega_h])^{t_n} + \int_{t_{n-1}}^{t_n} (\nabla U_h^\tau, [\nabla\omega - \nabla\omega_h])^{t_n}\\
&\qquad + ([\nabla U_h^\tau - \nabla u_h^n], \nabla\omega_h)^{t_n} - (\mathbf{Q}_h^\tau U_h^\tau, [\nabla\omega - \nabla\omega_h])^{t_n} - ([\mathbf{Q}_h^\tau - \mathbf{q}_h^n] U_h^\tau, \nabla\omega_h)^{t_n}\\
&\qquad - (\mathbf{Q}_h^\tau [U_h^\tau - u_h^n], \nabla\omega_h)^{t_n} + ([\mathbf{Q}_h^\tau - \mathbf{q}_h^n][U_h^\tau - u_h^n], \nabla\omega_h)^{t_n}\Big],\\
&(\partial_t V_h^\tau, \theta)^T \in (r(U_h^\tau) - H(V_h^\tau), \theta)^T + \textstyle\sum_{n=1}^N \Big[(\partial_t V_h^\tau, [\theta - \theta_h])^{t_n} - (r(U_h^\tau), [\theta-\theta_h])^{t_n}\\
&\quad - ([r(U_h^\tau) - r(u_h^{n-1})], \theta_h)^{t_n} + (H(V_h^\tau), [\theta - \theta_h])^{t_n} + ([H(V_h^\tau) - H(v_h^{n-1})], \theta_h)^{t_n}\Big].
\end{aligned}\right. \tag{46}$$

Note that, since $\mathcal{W}_h \in \ker C_h$, the terms in the equations for species transport that correspond to the hybrid inter-element variables can be eliminated, and the equations for (U_h^τ, V_h^τ) correspond to a primal formulation eventually converging to the continuous weak formulation (11) of Problem P_2. The equation for $(\mathbf{Q}_h^\tau, P_h^\tau, \Lambda_h^\tau)$ is a hybrid formulation on each element K, which eventually converges to a continuous dual mixed hybrid formulation, which is equivalent to the dual mixed formulation (11) of Problem P_2, since the continuous and the discrete quadratic forms are continuous and coercive over $\ker B$ and $\ker B_h$, and the continuous and the discrete inf–sup conditions are satisfied.

In order to pass to the limit in (46), for $h, \tau \to 0$, and identify the system satisfied by the limit points we need the following results.

Lemma 5. *The continuous interpolants satisfy*

$$\mathbf{Q}_h^\tau \in L^2\Big((0,T); \prod_{K\in\mathcal{T}_h} \boldsymbol{H}_{\mathrm{div}}(K)\Big) \cap L^\infty\Big((0,T); \prod_{K\in\mathcal{T}_h} L^2(K)\Big), \tag{47}$$

$$P_h^\tau \in L^\infty\Big((0,T); \prod_{K\in\mathcal{T}_h} L^2(K)\Big), \tag{48}$$

$$\Lambda_h^\tau \in L^\infty\Big((0,T); \prod_{K\in\mathcal{T}_h} L^2(\partial K)\Big), \tag{49}$$

$$U_h^\tau \in L^2((0,T); H_0^1(\Omega)) \cap L^\infty((0,T); L^2(\Omega)), \tag{50}$$

$$\partial_t U_h^\tau \in L^2((0,T); L^2(\Omega)), \tag{51}$$

$$V_h^\tau \in L^\infty((0,T); L^2(\Omega)), \tag{52}$$

$$\partial_t V_h^\tau \in L^2((0,T); L^2(\Omega)). \tag{53}$$

Proof. Consider the equation

$$\|\nabla U_h^\tau\|^2 = \|\nabla u_h^{n-1} + \nabla[u_h^n - u_h^{n-1}]\frac{t-t_{n-1}}{\tau}\|^2 \le 2\|\nabla u_h^{n-1}\|^2 + 2\frac{(t-t_{n-1})^2}{\tau^2}\|\nabla[u_h^n - u_h^{n-1}]\|^2.$$

We have, by integrating in time and using estimate (27), that

$$\begin{aligned}\int_0^T \|\nabla U_h^\tau\|^2 dt &\le 2\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\nabla u_h^{n-1}\|^2 + 2\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \frac{(t-t_{n-1})^2}{\tau^2}\|\nabla[u_h^n - u_h^{n-1}]\|^2 \\ &\le 2\tau\sum_{n=1}^N \|\nabla u_h^{n-1}\|^2 + \frac{2}{3}\tau\sum_{n=1}^N \|\nabla[u_h^n - u_h^{n-1}]\|^2 \le C.\end{aligned}$$

From this estimate we obtain (50) and (52). For what concerns the estimates on the time derivatives, we have that

$$\int_0^T \|\partial_t V_h^\tau\|^2 dt = \sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\frac{v_h^n - v_h^{n-1}}{\tau}\|^2 dt \le \sum_{n=1}^N \tau\|\frac{v_h^n - v_h^{n-1}}{\tau}\|^2 \le C,$$

thanks to (26). An estimate for $\|\partial_t U_h^\tau\|^2_{\Omega^T}$ is proved similarly and we obtain (51) and (53). We consider now the expression

$$\begin{aligned}\|\operatorname{div}\mathbf{Q}_h^\tau\|_K^2 &= \|\operatorname{div}\mathbf{Q}_h^{n-1} + \operatorname{div}[\mathbf{Q}_h^n - \mathbf{Q}_h^{n-1}]\frac{t-t_{n-1}}{\tau}\|_K^2 \\ &\le 2\|\operatorname{div}\mathbf{Q}_h^{n-1}\|_K^2 + 2\frac{(t-t_{n-1})^2}{\tau^2}\|\operatorname{div}[\mathbf{Q}_h^n - \mathbf{Q}_h^{n-1}]\|_K^2,\end{aligned}$$

which integrated in time, thanks to (32) and (33), provides

$$\int_0^T \| \operatorname{div} \mathbf{Q}_h^\tau \|_K^2 dt \leq C.$$

From this estimate and (28) and (29) we obtain (47), (48) and (49). □

We are now in the position of deriving the following convergence result.

Lemma 6 *(Convergence results). There exists a subsequence of continuous interpolants that, for $(h,\tau) \to 0$, satisfy*

$$\begin{aligned}
&U_h^\tau \rightharpoonup u \textit{ in } L^2((0,T); H_0^1(\Omega)),\\
&\partial_t U_h^\tau \rightharpoonup \partial_t u \textit{ in } L^2((0,T); H^{-1}(\Omega)),\\
&V_h^\tau \rightharpoonup v \textit{ in } L^2((0,T); L^2(\Omega)),\\
&\partial_t V_h^\tau \rightharpoonup \partial_t v \textit{ in } L^2((0,T); L^2(\Omega)),\\
&\mathbf{Q}_h^\tau \rightharpoonup \mathbf{q} \textit{ in } L^2\Bigg((0,T); \prod_{K\in\mathcal{T}_h} \boldsymbol{H}_{\operatorname{div}}(K)\Bigg),\\
&P_h^\tau \rightharpoonup p \textit{ in } L^2\Bigg((0,T); \prod_{K\in\mathcal{T}_h} L^2(K)\Bigg),\\
&\Lambda_h^\tau \rightharpoonup \lambda \textit{ in } L^2\Bigg((0,T); \prod_{K\in\mathcal{T}_h} H^{1/2}(\partial K)\Bigg) \hookrightarrow L^2\Bigg((0,T); \prod_{K\in\mathcal{T}_h} L^2(\partial K)\Bigg).
\end{aligned}$$

While,

$$U_h^\tau \to u \textit{ in } L^q(0,T; L^2(\Omega)), \forall q \geq 1.$$

Proof. The first set of results derive from (47)–(53), by the application of the Banach–Alaoglu theorem [24]. In particular, the convergence result for the sequence Λ_h^τ is given by its boundedness in the space $L^2((0,T); \prod_{K\in\mathcal{T}_h} H^{1/2}(\partial K))$, which is continuously embedded in $L^2((0,T); \prod_{K\in\mathcal{T}_h} L^2(\partial K))$. The boundedness in $L^2((0,T); \prod_{K\in\mathcal{T}_h} H^{1/2}(\partial K))$ can be obtained by extending Λ_h^τ from the edge to K by means of the lifting

$$\begin{cases} -\operatorname{div} \nabla \eta_h = P_h^\tau & \text{in} \quad K,\\ \eta_h|_{\partial K} = \Lambda_h^\tau, \end{cases} \tag{54}$$

using moreover (29) and standard results on elliptic regularity, trace theorems and interpolation spaces [1].

The last result is obtained thanks to compactness embedding, from the application of the method of the Hilbertian triad [24] and from the Lebesgue dominated convergence theorem. Indeed, thanks to (50) and (51) the set U_h^τ is relatively compact in $L^2(0,T; L^2(\Omega))$ and there exists a subsequence of U_h^τ which converges to the limit point u in $L^q(0,T; L^2(\Omega))$ $\forall q \geq 1$. □

The strong convergence of U_h^τ in $L^2(0,T; L^2(\Omega))$ makes it possible to pass to the limit in the nonlinear term $r(U_h^\tau)$ of equation (46).

Note that the family of functions V_h^τ is only weakly convergent to a limit point in $L^2(0,T; L^2(\Omega))$. This is not a problem when passing to the limit in terms like $\int_0^T (H(V_h^\tau), \theta) \to \int_0^T (H(v), \theta)$, because of the properties of the multivalued map H. Namely, the set $H(V_h^\tau)$ is bounded and convex, so it is weakly closed. Hence it is weakly compact, and admits a weakly convergent subsequence: $\lim_{(h,\tau)}(H(V_h^\tau),\theta) \to (H(v),\theta)$. Moreover, since V_h^τ is weakly convergent in $L^2(0,T;L^2(\Omega))$ and using the upper semicontinuity and the maximal monotonicity property of the multivalued map H, we have that $\lim_{(h,\tau)}\int_0^T (H(V_h^\tau),\theta) = \int_0^T \lim_{(h,\tau)}(H(V_h^\tau),\theta)$. This would be sufficient if we were solving the problem with a given Darcy flux: solving directly the inclusion problem without regularization avoids the necessity of strong convergence of V_h^τ in $L^2(0,T;L^2(\Omega))$. Since however we are considering the coupling with a Darcy field, in order to pass to the limit in terms containing the non-linear permeability factor $[k_\epsilon(V_h^\tau)]^{-1}$ we need strong convergence. We obtain it in the following lemma.

Lemma 7. *$V_h^\tau \to v$ in $L^2(0,T;L^2(\Omega))$.*

Proof. The proof is the same as that introduced in [15] in Proposition 4.6 and Lemma 4.7. The only difference here is that, instead of a Lipschitz continuous regularization of the dissolution rate, we have a semicontinuous rate, satisfying the selection (6). Here we only report the generalization of the result proved in Proposition 4.6 to this particular case. Remembering that $v_h \in \mathcal{W}_h$ and using (6), the result in Proposition 4.6 becomes

$$\|\nabla P_K^1 H(v_h)\|_K \le L_r \|\nabla u_h\|_K,$$

where L_r is the Lipschitz constant of the function $r(\cdot)$. We refer to [15] for the details of the proof. □

We finally investigate the limit equations of system (46) for $(\tau,\, h) \to 0$.

Theorem 4. *The limit point $(\mathbf{q},\, p,\, \lambda,\, u,\, v)$ is the weak solution of a hybrid formulation of the weak Problem P_2, which is equivalent to the weak solution of Problem P_2.*

Proof. Let us start from considering the first equation of system (46). The left hand side converges to the limit

$$\int_0^T \left(\frac{\mu}{k_\epsilon(v)}\mathbf{q},\boldsymbol{\tau}\right)_K dt - \int_0^T (p, \operatorname{div}\boldsymbol{\tau})_K dt + \int_0^T (\lambda, \boldsymbol{\tau}\cdot\mathbf{n})_{\partial K} + \int_0^T (p_D, \boldsymbol{\tau}\cdot\mathbf{n})_{\partial K\cap\Gamma_D}.$$

For all but the first term this is a direct consequence of the convergence results (47), (48) and (49). The first term can be rewritten as

$$\int_0^T \left(\frac{\mu}{k_\epsilon(V_h^\tau)}\mathbf{Q}_h^\tau,\boldsymbol{\tau}\right)_K dt = \int_0^T \left(\frac{\mu}{k_\epsilon(v)}\mathbf{Q}_h^\tau,\boldsymbol{\tau}\right)_K dt + \int_0^T \left(\left[\frac{\mu}{k_\epsilon(V_h^\tau)} - \frac{\mu}{k_\epsilon(v)}\right]\mathbf{Q}_h^\tau,\boldsymbol{\tau}\right)_K dt.$$

Since $V_h^\tau \to v$ strongly and is in $L^\infty(\Omega)$, and since $\mathbf{Q}_h^\tau$ is weakly convergent in $L^2(0,T;L^2(\Omega))$, the first term on the right hand side converges to the desired limit. Choosing a test function $\boldsymbol{\tau} \in L^2(0,T;[C_0^\infty(\Omega)]^2)$, we can show that the second term on the right hand side is zero by bounding it using the estimate

$$\begin{aligned}\int_0^T \left(\left[\frac{\mu}{k_\epsilon(V_h^\tau)} - \frac{\mu}{k_\epsilon(v)}\right]\mathbf{Q}_h^\tau,\boldsymbol{\tau}\right)_K dt &\le \left\|\left[\frac{\mu}{k_\epsilon(V_h^\tau)} - \frac{\mu}{k_\epsilon(v)}\right]\mathbf{Q}_h^\tau\right\|_{[L^1(\Omega)]^2} \\ &\le C\|V_h^\tau - v\|_{[L^2(\Omega)]^2}\|\mathbf{Q}_h^\tau\|_{L^2(\Omega)} \to 0,\end{aligned}$$

where we have used the Lipschitz continuity of the function $[k_\epsilon(\cdot)]^{-1}$ and the fact that $V^\tau_h \to v$ in the $L^2(\Omega)$ norm. Hence, the left hand side of the first equation of system (46) converges in the distributional sense to the continuous hybrid formulation, extended to Ω, of the first equation of Problem P_2.

We now show that the terms in the right hand side of the first equation of system (46) converge to zero for $(h,\tau) \to 0$. Let us denote these terms by $\mathcal{I}_1, \cdots, \mathcal{I}_9$. Considering estimate (47) and the first interpolation estimate of (24), we conclude that

$$|\mathcal{I}_1| \leq C\Big(\int_0^T \|\mathbf{Q}_h^\tau\|_K^2 dt\Big)^{1/2}\Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\boldsymbol{\tau} - \boldsymbol{\tau}_h\|_K^2 dt\Big)^{1/2} \leq Ch\|\boldsymbol{\tau}\|_{L^2(0,T;\prod_{K\in\mathcal{T}_h}[H^1(K)]^2)} \to 0.$$

Considering the first estimate in (26), the estimate (47), the Lipschitz continuity property of the function $[k_\epsilon(\cdot)]^{-1}$, recalling that $\|\operatorname{div}\mathbf{Q}_h^\tau\|_K = \|\nabla\mathbf{Q}_h^\tau\|_K$ and $\|\operatorname{div}\boldsymbol{\tau}_h\|_K = \|\nabla\boldsymbol{\tau}_h\|_K$, and applying a trilinear Hölder inequality, we obtain

$$\begin{aligned}|\mathcal{I}_2| &\leq C\Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|v_h^n - v_h^{n-1}\|_K^2 \|\operatorname{div}\mathbf{Q}_h^\tau\|_K^2 dt\Big)^{1/2}\Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\nabla\boldsymbol{\tau}_h\|_K^2 dt\Big)^{1/2} \\ &\leq C\Big(\sum_{n=1}^N \tau^3\|\operatorname{div}\mathbf{Q}_h^\tau\|_K^2\Big)^{1/2}\Big(\sum_{n=1}^N \tau\|\nabla\boldsymbol{\tau}_h\|_K^2\Big)^{1/2} \to 0.\end{aligned}$$

While, by considering estimate (30), we get

$$|\mathcal{I}_3| \leq C\Big(\sum_{n=1}^N \tau\|\mathbf{q}_h^n - \mathbf{q}_h^{n-1}\|_K^2\Big)^{1/2}\Big(\sum_{n=1}^N \tau\|\boldsymbol{\tau}_h\|_K^2\Big)^{1/2} \to 0.$$

Thanks to the first estimate in equation (26), estimate (33), and by applying a trilinear Hölder inequality, we are able to write

$$\begin{aligned}|\mathcal{I}_4| &\leq C\Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|v_h^n - v_h^{n-1}\|_K^2 \|\operatorname{div}[\mathbf{q}_h^n - \mathbf{q}_h^{n-1}]\|_K^2 dt\Big)^{1/2}\Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\nabla\boldsymbol{\tau}_h\|_K^2 dt\Big)^{1/2} \\ &\leq C\Big(\sum_{n=1}^N \tau^3\|\operatorname{div}[\mathbf{q}_h^n - \mathbf{q}_h^{n-1}]\|_K^2\Big)^{1/2}\Big(\sum_{n=1}^N \tau\|\nabla\boldsymbol{\tau}_h\|_K^2\Big)^{1/2} \to 0.\end{aligned}$$

Considering (29) and the second interpolation estimate in (24), we get

$$|\mathcal{I}_5| \leq C\Big(\int_0^T \|P_h^\tau\|_K^2 dt\Big)^{1/2}\Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\operatorname{div}[\boldsymbol{\tau} - \boldsymbol{\tau}_h]\|_K^2 dt\Big)^{1/2} \leq Ch\|\boldsymbol{\tau}\|_{L^2(0,T;\prod_{K\in\mathcal{T}_h}[H^2(K)]^2)} \to 0.$$

Note that for this estimate we need to restrict the test functions to be in $L^2(0,T;\prod_{K\in\mathcal{T}_h}[H^2(K)]^2)$. Density arguments ensure that the limit points satisfy the continuous weak formulation also for $\boldsymbol{\tau} \in L^2(0,T;\prod_{K\in\mathcal{T}_h}[H^1(K)]^2)$. Thanks to the first estimate in (31), we have

$$\begin{aligned}|\mathcal{I}_6| &\leq C\Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|p_h^n - p_h^{n-1}\|_K^2 dt\Big)^{1/2}\big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\operatorname{div}\boldsymbol{\tau}_h\|_K^2 dt\big)^{1/2} \\ &\leq C\Big(\sum_{n=1}^N \tau\|p_h^n - p_h^{n-1}\|_K^2\Big)^{1/2}\Big(\sum_{n=1}^N \tau\|\operatorname{div}\boldsymbol{\tau}_h\|_K^2\Big)^{1/2} \to 0.\end{aligned}$$

Considering the second estimate in equation (30) and the sixth interpolation estimate of (24) we obtain in a similar manner that $|\mathcal{I}_7| \to 0$, $|\mathcal{I}_8| \to 0$ and $|\mathcal{I}_9| \to 0$.

Let us consider now the second equation of system (46). The left hand side converges to

$$\int_0^T (\operatorname{div} \mathbf{q}, \psi)_K dt - \int_0^T (\partial_t v, \psi)_K dt,$$

as a direct consequence of the convergence results in (47) and (53). We now show that the terms in the right hand side converge to zero for $(h,\tau) \to 0$. Let us denote these terms by the notation $\mathcal{I}_1, \cdots, \mathcal{I}_3$. Using (47) and the third interpolation estimate of (24), we have

$$|\mathcal{I}_1| \leq \left(\int_0^T \| \operatorname{div} \mathbf{Q}_h^\tau \|_K^2 dt \right)^{1/2} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\psi - \psi_h\|_K^2 dt \right)^{1/2} \leq Ch \|\psi\|_{L^2(0,T;\prod_{K\in\mathcal{T}_h} H^1(K))} \to 0.$$

Note that we are again restricting the test functions to $L^2(0,T;H^1(K))$; density arguments extend the result to $\psi \in L^2(0,T;L^2(\Omega))$. Estimate (33) allows us to write

$$|\mathcal{I}_2| \leq \left(\sum_{n=1}^N \tau \| \operatorname{div}[\mathbf{q}_h^n - \mathbf{q}_h^{n-1}] \|_K^2 \right)^{1/2} \left(\sum_{n=1}^N \tau \|\psi_h\|_K^2 \right)^{1/2} \to 0.$$

Considering estimate (53) and the third interpolation estimate of (24), we also have that

$$|\mathcal{I}_3| \leq \left(\int_0^T \|\partial_t V_h^\tau\|_K^2 dt \right)^{1/2} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\psi - \psi_h\|_K^2 dt \right)^{1/2} \leq Ch \|\psi\|_{L^2(0,T;\prod_{K\in\mathcal{T}_h} H^1(K))} \to 0.$$

For what concerns the third equation of system (46), the left hand side converges to the limit

$$\int_0^T (\mathbf{q} \cdot \mathbf{n}, \rho)_{\partial K} dt.$$

This is a direct consequence of the convergence result in (47). We now show that the terms in the right hand side converge to zero for $(h,\tau) \to 0$. Let us denote these terms by the notation $\mathcal{I}_1, \mathcal{I}_2$. Using estimate (47) and the fifth interpolation estimate of (24) we have that

$$|\mathcal{I}_1| \leq \left(\int_0^T \|\mathbf{Q}_h^\tau \cdot \mathbf{n}\|_K^2 dt \right)^{1/2} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\rho - \rho_h\|_{\partial K}^2 dt \right)^{1/2} \leq Ch \|\rho\|_{L^2(0,T;\prod_{K\in\mathcal{T}_h} H^{3/2}(K))} \to 0.$$

The term $|\mathcal{I}_2| = 0$, since $\rho_h \in \mathcal{P}_h$.

Let us proceed with the fourth equation of system (46). The left hand side converges to the limit

$$\int_0^T (\partial_t u, \phi) dt + \int_0^T (\nabla u, \nabla \phi) dt - \int_0^T (\mathbf{q} u, \nabla \phi) dt + \int_0^T (\partial_t v, \phi) dt.$$

For all but the third term this is a direct consequence of the convergence results (50), (51) and (53). The third term can be rewritten as

$$\int_0^T (\mathbf{Q}_h^\tau U_h^\tau, \nabla\phi)dt = \int_0^T (\mathbf{q} U_h^\tau, \nabla\phi)dt + \int_0^T ([\mathbf{Q}_h^\tau - \mathbf{q}]U_h^\tau, \nabla\phi)dt.$$

Since $\mathbf{Q}_h^\tau \to \mathbf{q}$ strongly in $[L^2(\Omega)]^2$, and since U_h^τ is weakly convergent in $L^2(0,T;H_0^1(\Omega))$, the term on the right hand side converges to the desired limit. The second term on the right hand side is zero, since $U_h^\tau \in L^\infty(\Omega)$ and $\mathbf{Q}_h^\tau \to \mathbf{q}$ strongly in $[L^2(\Omega)]^2$. Hence, the left hand side of the fourth equation of system (46) converges in the distributional sense to the fourth equation of Problem P_2.

We now show that the terms in the right hand side converge to zero for $(h,\tau) \to 0$. Let us denote these terms by the notation $\mathcal{I}_1, \cdots, \mathcal{I}_8$. Thanks to (51) and the fourth interpolation estimate in (24), we may write

$$|\mathcal{I}_1| \leq \Big(\int_0^T \|\partial_t U_h^\tau\|^2 dt\Big)^{1/2} \Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\phi - \phi_h\|^2 dt\Big)^{1/2} \leq Ch\|\phi\|_{L^2(0,T;H_0^1(\Omega))} \to 0.$$

Similarly, we obtain $|\mathcal{I}_2| \to 0$ by considering estimate (53), and the fourth interpolation estimate of (24). Using (50) and the fourth interpolation estimate in (24) we can write

$$|\mathcal{I}_3| \leq \Big(\int_0^T \|\nabla U_h^\tau\|^2 dt\Big)^{1/2} \Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\nabla\phi - \nabla\phi_h\|^2 dt\Big)^{1/2} \leq Ch\|\phi\|_{L^2(0,T;H^2(\Omega))} \to 0.$$

Note that we have to restrict the test functions to $\phi \in L^2(0,T;H^2(\Omega))$. Density arguments ensure that the limit points satisfy the continuous weak formulation also for $\phi \in L^2(0,T;H_0^1(\Omega))$. Considering (27), we have that

$$|\mathcal{I}_4| \leq \Big(\sum_{n=1}^N \tau\|\nabla u_h^n - \nabla u_h^{n-1}\|^2\Big)^{1/2} \Big(\sum_{n=1}^N \tau\|\nabla\phi_h\|^2\Big)^{1/2} \to 0.$$

Thanks to estimate (47) and the fourth interpolation estimate in (24), we obtain

$$|\mathcal{I}_5| \leq C\Big(\int_0^T \|\mathbf{Q}_h^\tau\|^2 dt\Big)^{1/2} \Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\nabla\phi - \nabla\phi_h\|^2 dt\Big)^{1/2} \leq Ch\|\phi\|_{L^2(0,T;H^2(\Omega))} \to 0.$$

While, by using (30),

$$|\mathcal{I}_6| \leq C\Big(\sum_{n=1}^N \tau\|\mathbf{q}_h^n - \mathbf{q}_h^{n-1}\|^2\Big)^{1/2} \Big(\sum_{n=1}^N \tau\|\nabla\phi_h\|^2\Big)^{1/2} \to 0.$$

This bound can be used in a similar way to show that $|\mathcal{I}_8| \to 0$. The second part of (26) and the estimate (47) allow us to state that

$$|\mathcal{I}_7| \leq C\Big(\sum_{n=1}^N \tau\|u_h^n - u_h^{n-1}\|^2\Big)^{1/2} \Big(\sum_{n=1}^N \tau\|\nabla\phi_h\|^2\Big)^{1/2} \to 0.$$

Finally, we consider the fifth equation in (46). The left hand side converges to

$$\int_0^T (\partial_t v, \theta) dt \in \int_0^T (r(u) - H(v), \theta) dt.$$

This is a direct consequence of the convergence results (50) and (51) (which imply strong convergence of U_h^τ), equation (53) and the properties of the map $H(\cdot)$. Hence, the left hand side of the fifth equation of system (46) converges in the distributional sense to the fifth equation of Problem P_2. For what concerns the terms in the right hand side, let us denote them by the notation $\mathcal{I}_1, \cdots, \mathcal{I}_5$. We have already demonstrated that $\mathcal{I}_1 \to 0$ if $\theta \in L^2(0,T;H_0^1(\Omega))$. Exploiting the Lipschitz continuity of the function $r(\cdot)$, estimate (50) and the fourth interpolation estimate in (24), we get

$$|\mathcal{I}_2| \le L_r \Big(\int_0^T \|U_h^\tau\|^2 dt\Big)^{1/2} \Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\theta - \theta_h\|^2 dt\Big)^{1/2} \le Ch\|\theta\|_{L^2(0,T;H_0^1(\Omega))} \to 0.$$

While, thanks to the Lipschitz continuity of $r(\cdot)$ and the second part of the estimate (26),

$$|\mathcal{I}_3| \le L_r \Big(\sum_{n=1}^N \tau \|u_h^n - u_h^{n-1}\|^2\Big)^{1/2} \Big(\sum_{n=1}^N \tau \|\theta_h\|^2\Big)^{1/2} \to 0.$$

The boundedness of the map $H(\cdot)$ allows us to write

$$|\mathcal{I}_4| \le C \Big(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\theta - \theta_h\|^2 dt\Big)^{1/2} \le Ch\|\theta\|_{L^2(0,T;H_0^1(\Omega))} \to 0.$$

Finally, thanks to the Filippov selection method, we have that $\|H(V_h^\tau) - H(v_h^{n-1})\| \le L_r \|u_h^n - u_h^{n-1}\|$ (note that if $v_h^{n-1} = 0$, then also $v_h^n = 0$). Hence, $|\mathcal{I}_5| \le |\mathcal{I}_3| \to 0$. Which provides the last result and completes the proof. □

3. A numerical example

In this section we present a test case concerning the numerical solution of Problem P_2^h. There are three basic ways of solving discontinuous differential problems. The first is to eliminate the discontinuity by using a suitable smoothing operator, which typically depends on a single parameter. The main limitation of this approach is that the solution depends on the value of the parameter and a compromise must be set between accuracy and stiffness of the regularized problem. A second technique consists in simply ignoring the discontinuity and relying on adaptive stepping schemes. The error indicator associated to several time advancing scheme will detect the discontinuity and refine the step in its vicinity. The drawback here is that the refinement may be extremely fine, with the resulting computational cost, and it may be difficult to maintain the order of accuracy. Moreover, both techniques may fail, or give unsatisfactory results, in the case of sliding motion, i.e. when the solution after reaching the discontinuity surface, slides onto it [6]. A third approach is based on detecting when the solution reaches the discontinuity and select its behavior according to Filippov theory [9]. These methods, often called event driven methods, may guarantee optimal convergence at reasonable computational cost, and allow for the resolution of sliding motions. We employ a numerical procedure based on the event driven method for DRH systems [8], applied to the Euler explicit scheme in (25): this time-discrete scheme decouples the transport from the reaction and the Darcy terms. At each time step n we advance in time with the reaction term. If the trajectory meets the discontinuity surface at an instant t^* inside the current time step, we localize the intersection between the trajectory and the surface and restart the integration from t^*, after having selected the corresponding element of the set $H(v_h)$ according to the Filippov prescription (6). The Darcy equations are then solved by static condensation, and the Darcy field is used inside the advection–diffusion–reaction equation for u_h^{n+1}. We compare the results obtained by the application of the event driven method with those obtained by the regularization approach of the right hand side introduced in [15], which is given by representing the Heaviside function through a linear interpolation

$$H_\delta(v) = \begin{cases} 0 & \text{if} \quad v \leq 0, \\ v/\delta & \text{if} \quad 0 \leq v \leq \delta, \\ 1 & \text{if} \quad v > \delta, \end{cases}$$

where δ is a small positive parameter which, in order to guarantee the convergence property of the discrete scheme to the continuous weak solution, must satisfy the condition $\delta = O(\Delta t^a)$, for some $0 < a < 1$. The problem is set in a square 2D domain $\Omega := (0,1) \times (0,1)$, with a Dirichlet boundary $\Gamma_D := \{y : \ x = 0, \ y \in (0,1)\}$ and $\Gamma_N := \partial\Omega \setminus \Gamma_D$. Moreover, the viscosity is set to $\mu = 1$ and precipitation is modeled as $r(u) = u$. We set the following initial conditions:

$$u|_{t=0} = 1 \quad \text{in } (x,y) \in \Omega,$$
$$v|_{t=0} = \begin{cases} 0.8 & \text{in } (x,y) \in \Omega_v, \\ 0 & \text{in } (x,y) \in \Omega \setminus \Omega_v, \end{cases}$$

where $\Omega_v \subset \Omega$, $\Omega_v := \{(x,y) : \ 0.4 \leq x \leq 0.6, \ 0.4 \leq y \leq 0.6\}$, and solve Problem P_2^h on the time interval $t \in [0,1]$, with a time step $\Delta t = 0.01$. We choose two different values for the positive parameter δ: a small value $\delta = 0.005$ with respect to Δt, and a value $\delta = \Delta t^{1/2} = 0.1$, which satisfies the condition $\delta = O(\Delta t^a)$ introduced in [15]. We set $\Gamma_1 := \{y : x = 0, \ y \in (0,1)\}$, $\Gamma_2 := \{x : y = 0, \ x \in (0,1)\}$, $\Gamma_3 := \{y : x = 1, \ y \in (0,1)\}$ and $\Gamma_4 := \{x : y = 1, \ x \in (0,1)\}$, and $p = 0.5, u = 0$ on Γ_1, $p = 0, \nabla u \cdot \mathbf{n} = 0$ on Γ_3, $\mathbf{q} \cdot \mathbf{n} = 0, \nabla u \cdot \mathbf{n} = 0$ on $\Gamma_2 \cup \Gamma_4$. The domain is discretized with a structured triangular grid of 10 000 elements.

The evolution of cation and precipitate concentrations and magnitude of the Darcy velocity are represented in Fig. 1, both for the cases of the application of the event driven method and the regularization approach with a small value $\delta = 0.005$. The solution exhibits an attractive sliding motion on the discontinuity of the Heaviside function in $\Omega \setminus \Omega_v$, where, as a consequence, the precipitate concentration v remains constant and equal to 0. Note that the regularization approach fails at representing correctly the sliding motion on $v = 0$. This is due to the fact that, being $\Delta t > \delta$ (which violates the requirement $\delta = O(\Delta t^a)$ introduced in [15]), the solution can exceed the threshold value and start oscillating around it. This causes spurious oscillations in the time evolution of the magnitude of the Darcy field as well. In Fig. 2 we show the evolution of the difference between the cation concentration values calculated with the event driven and the regularization with $\delta = 0.005$ methods (u DRH–u Smooth), and between the precipitate concentration values calculated with the two methods (v DRH–v Smooth). We can note that, after the first time step, (at time $t = 0.01$ [s]), the regularization approach exceeds the threshold value by a quantity equal to 2δ. The oscillations around the threshold value decrease in time, and the concentration values calculated with the regularization method approach those calculated with the event driven method as time advances.

In Fig. 3 we show the evolution of cation and precipitate concentrations and magnitude of the Darcy velocity for the case of the application of the regularization approach with a $\delta = \Delta t^{1/2} = 0.1$. In this case the precipitate concentration v exits the sliding motion on the discontinuity of the Heaviside function in $\Omega \setminus \Omega_v$, due to the wide thickness of the regularization layer in $H_\delta(v)$. Better results would be produced by

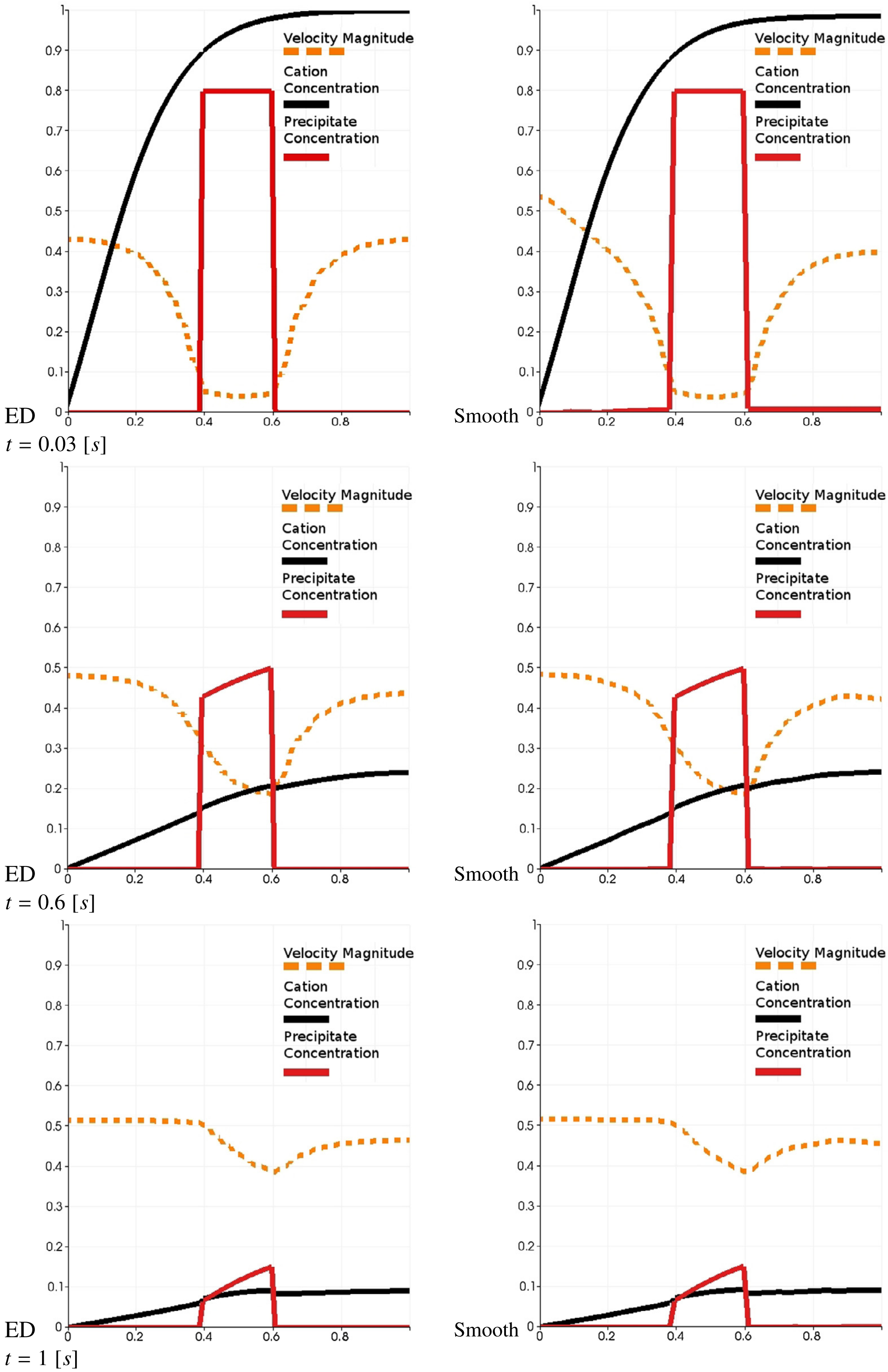

Fig. 1. Cation concentration (u), precipitate concentration (v) and velocity magnitude $|\mathbf{q}|$ at times 0.03 [s], 0.6 [s], 1 [s], in the case of the application of event driven method (ED) and regularization approach with $\delta = 0.005$ (Smooth).

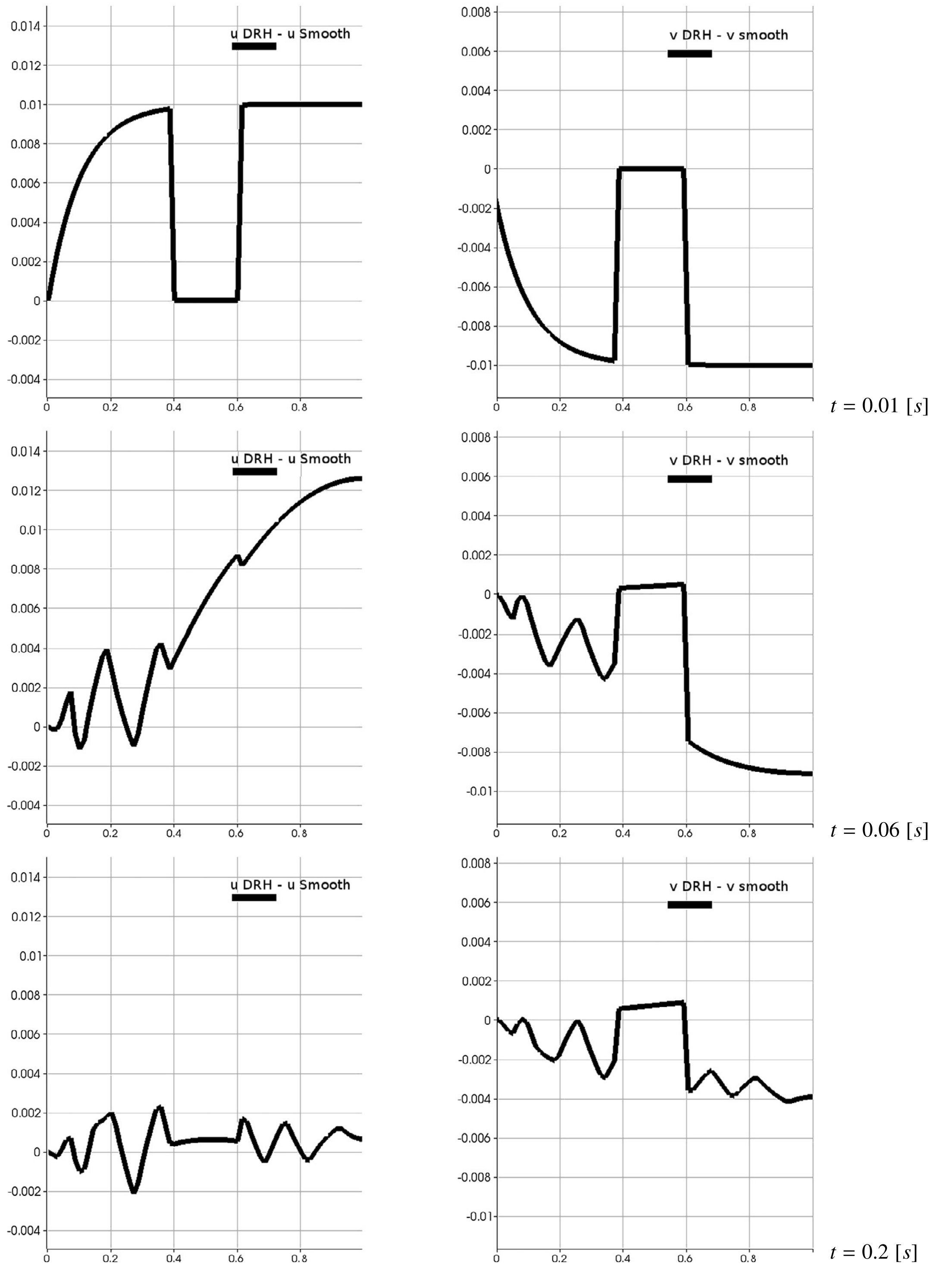

Fig. 2. Difference between the cation concentration values calculated with the event driven and the regularization with $\delta = 0.005$ methods (u DRH–u Smooth), and between the precipitate concentration values calculated with the event driven and the regularization methods (v DRH–v Smooth), at times 0.01 [s], 0.06 [s], 0.2 [s].

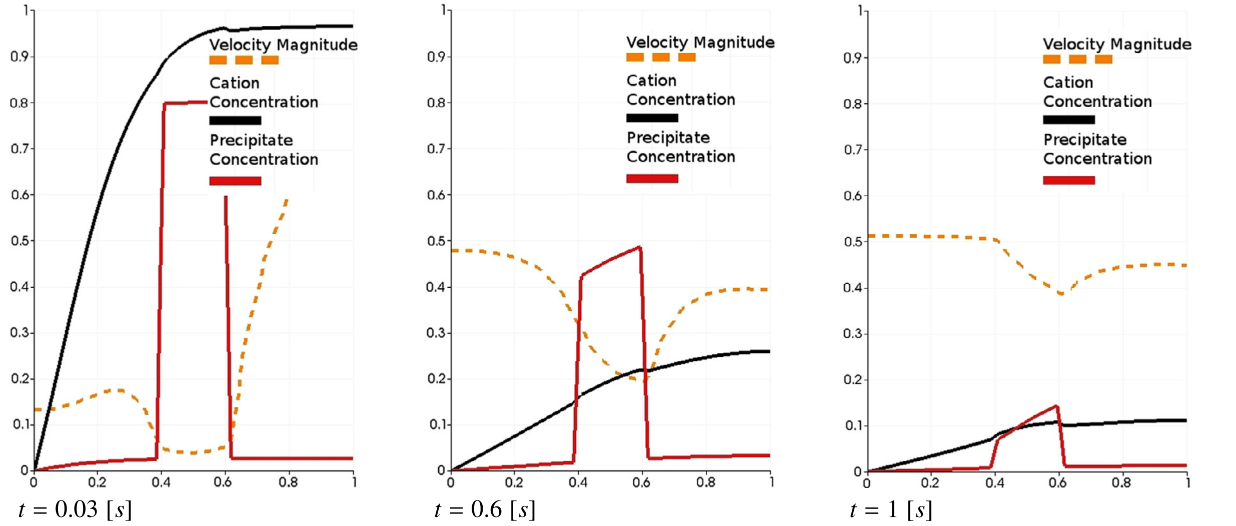

Fig. 3. Cation concentration (u), precipitate concentration (v) and velocity magnitude $|\mathbf{q}|$ at times 0.03 [s], 0.6 [s], 1 [s], in the case of the application of the regularization approach with $\delta = \Delta t^{1/2} = 0.1$.

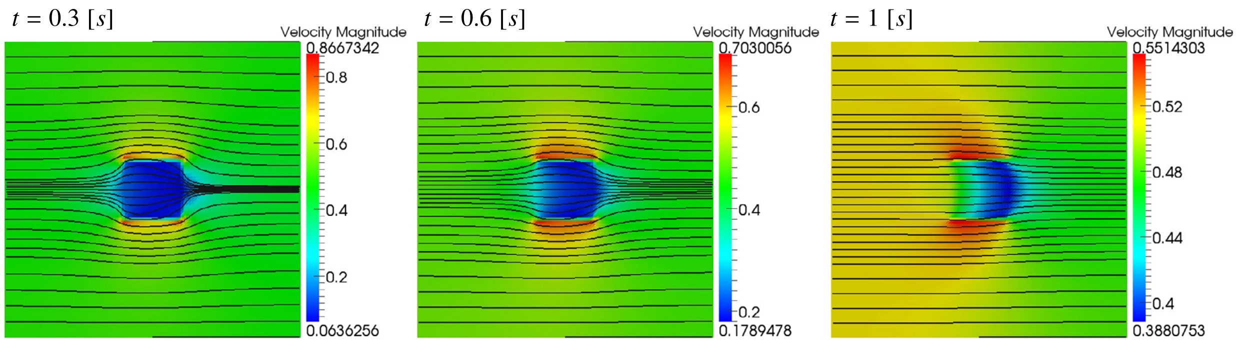

Fig. 4. Streamlines and magnitude of the velocity field $\mathbf{q}$ at times 0.3 [s], 0.6 [s], 1 [s], in the case of the application of event driven method.

considering smaller values of Δt, at the same time maintaining the requirement that $\delta = O(\Delta t^a)$. We thus conclude that the event driven method gives good results without requiring to decrease the value of Δt.

The dependence of the numerical solutions on the ratio between Δt and δ, and the order of convergence of event driven and regularized methods for explicit and implicit first order and higher order schemes will be studied in more detail in a forthcoming work.

The magnitude of the Darcy velocity $\mathbf{q}$ and its streamlines are reported in Fig. 4, for the case of the event driven method. The decrease of cation concentration u causes dissolution in Ω_v. The variation of v corresponds to a porosity change, and, consequently, to a change in the permeability in time. It can be noted that the velocity $\mathbf{q}$ increases in Ω_v as the precipitate dissolves. The streamlines superimposed in Fig. 4 show that the precipitate concentration forms at the beginning of the simulation an obstacle for the flow that is then gradually eroded.

4. Conclusion

In this paper we have shown for the first time the well-posedness of a simple model for dissolution–precipitation coupled with Darcy flow. We have treated the presence of thresholds in the reaction term without resorting to regularization. This has led to a problem that may be cast as differential inclusion.

We think that this result is rather important since it gives ground to event-driven numerical schemes for this class of problems that are able to properly treat the thresholds and allow to maintain the order in time of the basic scheme used for numerical integration. Even if we have used a very simple model for the dissolution process, numerical tests, which are the subject of forthcoming work, show that the technique of treating thresholds as discontinuities without regularization is not only a viable solution, but in several cases provides an effective numerical tool capable of giving accurate results in an efficient way.

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