

# Convergence analysis of mixed numerical schemes for reactive in a porous medium

*Citation for published version (APA):* Kumar, K., Pop, I. S., & Radu, F. A. (2012). *Convergence analysis of mixed numerical schemes for reactive in a porous medium*. (CASA-report; Vol. 1220). Technische Universiteit Eindhoven.

Document status and date: Published: 01/01/2012

#### Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

#### Please check the document version of this publication:

• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.

• The final author version and the galley proof are versions of the publication after peer review.

• The final published version features the final layout of the paper including the volume, issue and page numbers.

Link to publication

#### General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- · Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
  You may freely distribute the URL identifying the publication in the public portal.

If the publication is distributed under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license above, please follow below link for the End User Agreement:

www.tue.nl/taverne

#### Take down policy

If you believe that this document breaches copyright please contact us at:

openaccess@tue.nl

providing details and we will investigate your claim.

### EINDHOVEN UNIVERSITY OF TECHNOLOGY

Department of Mathematics and Computer Science

CASA-Report 12-20 June 2012

Convergence analysis of mixed numerical schemes for reactive flow in a porous medium

by

K. Kumar, I.S. Pop, F.A. Radu



Centre for Analysis, Scientific computing and Applications Department of Mathematics and Computer Science Eindhoven University of Technology P.O. Box 513 5600 MB Eindhoven, The Netherlands ISSN: 0926-4507

### CONVERGENCE ANALYSIS OF MIXED NUMERICAL SCHEMES FOR REACTIVE FLOW IN A POROUS MEDIUM

K. KUMAR  $^1$  , I. S.  $\mathrm{POP}^{1,2}$  , F. A. RADU  $^2$ 

<sup>1</sup> CASA, TECHNISCHE UNIVERSITEIT EINDHOVEN, EINDHOVEN, THE NETHERLANDS <sup>2</sup> INSTITUTE OF MATHEMATICS, JOHANNES BRUNS GT. 12, UNIVERSITY OF BERGEN,

NORWAY

**Abstract.** This paper deals with the numerical analysis of an upscaled model describing the reactive flow in a porous medium. The solutes are transported by advection and diffusion and undergo precipitation and dissolution. The reaction term and, in particular, the dissolution term has a particular, multi-valued character, which leads to stiff dissolution fronts. We consider the Euler implicit method for the temporal discretization and the mixed finite element for the discretization in time. More precisely, we use the lowest order Raviart-Thomas elements. As an intermediate step we consider also a semi-discrete mixed variational formulation (continuous in space). We analyse the numerical schemes and prove the convergence to the continuous formulation. Apart from the proof for the convergence, this also yields an existence proof for the solution of the model in mixed variational formulation. Numerical experiments are performed to study the convergence behavior.

 ${\bf Key}$  words. Numerical analysis, reactive flows, weak formulation, implicit scheme, mixed finite element discretization

#### AMS subject classifications. 35A35, 65L60, 65J20

1. Introduction. Reactive flows in a porous medium have a wide range of applications ranging from spreading of polluting chemicals leading to ground water contamination (see [41] and references therein) to biological applications such as tissue and bone formation, or pharmaceutical applications [27] or technological applications such as operation of solid batteries. A common feature of the above applications is the transport and reactions of ions/solutes. In this work, we deal with the transport of ions/solutes taking place through the combined process of convection and diffusion. For reactions, we focus on a specific class, namely the precipitation and dissolution processes, where the ions undergo combination (precipitation) to form a crystal. The reverse process of dissolution takes place where the crystal gets dissolved.

In this work, we consider an upscaled model defined on a Darcy scale. This implies that the solid grains and the pore space are not distinguished and the equations are defined everywhere. Consequently, the crystals formed as a result of reactions among ions and the ions themselves are defined everywhere in the domain. Such models fall in the general category of reactive porous media flow models. For Darcy-scale models related directly to precipitation and dissolution processes we refer to [7, 29, 33, 34] (see also the references therein). Here we adopt the ideas proposed first in [23], and extended in a series of papers [15, 16, 17]. These papers are referring to Darcy scale models; the porescale counterpart is considered in [18], where distinction is made for the domains delineating the pore space and the solid grains. The transition from the porescale model to the upscaled model is obtained, for instance, via homogenization arguments. For a simplified situation of a 2D strip, the rigorous arguments are provided in [18]; see also [28, 1] for the upscaling procedure in transport dominated flow regimes. For a similar situation, but tracking the geometry changes due to the reactions leading to the free boundary problems, the formal arguments are presented in [24] and [30].

We are motivated by analyzing appropriate numerical methods for solving the reactive flows for an upscaled model. Considering the mixed variational formulation is an attractive proposition as it preserves the mass locally. Our main goal here is to provide the convergence of a mixed finite element discretization for such a model for dissolution and precipitation in porous media, involving a multi-valued dissolution rate. Before discussing the details and specifics, we briefly review some of the relevant numerical work. For continuously differentiable rates the convergence of (adaptive) finite volume discretizations is studied in [22, 32]; see also [10] for the convergence of a finite volume discretization of a copper-leaching model. In a similar framework, discontinuous Galerkin methods are discussed in [40] and upwind mixed FEM are considered in [11, 12];

#### Kumar, Pop, and Radu

combined finite volume-mixed hybrid finite elements are employed in [20, 21]. Non-Lipschitz, but Hölder continuous rates are considered using conformal FEM schemes in [4, 5]. Similarly, for Hölder continuous rates (including equilibrium and non-equilibrium cases) mixed FEM methods are analyzed rigorously in [36, 39], whereas [37] provides error estimates for the coupled system describing unsaturated flow and reactive transport. In all these cases, the continuity of the reaction rates allows obtaining error estimates. A characteristic mixed-finite element method for the advection dominated transport has been treated in [3] and characteristic FEM scheme for contaminant transport giving rise to possibly non-Lipschitz reaction rates are treated in [13] where the convergence and the error estimates have been provided. A parabolic problem coupled with linear ODEs at the boundary have been treated in [2] using characteristic MFEM method. Conformal schemes both for the semi-discrete and fully discrete (FEM) cases for the upscaled model under consideration have been treated in [26].

The main difficulty here is due to the particular description of the dissolution rate involving differential inclusions. To deal with this, we consider a regularization of this term and the corresponding sequence of regularized equations. The regularization parameter  $\delta$  is dependent on the time discretization parameter  $\tau$  in such a way that as  $\tau \searrow 0$ , it is ensured that  $\delta \searrow 0$ . Thus, obtaining the limit of discretized scheme automatically yields, by virtue of the regularization parameter also vanishing, the original equation. In proving the convergence results, the compactness arguments are employed. These arguments rely on a priori estimates providing weak convergence. However, strong convergence is needed to deal with the non-linear terms in the reaction rates. Translation estimates are used to achieve this.

We consider both the semi-discrete and the fully discrete cases with the proof for the latter case following closely the ideas of semi-discrete case. However, there are important differences particularly in the way the translation estimates are obtained. Whereas in the semi-discrete case, we use the dual problem for obtaining the translation estimates; in the fully discrete case, we use the properties of discrete  $H_0^1$  norm following the finite volume framework [19]. The convergence analysis of appropriate numerical schemes for the problem considered here is a stepping stone for coupled flow and reactive transport problem (for example, Richards' equation coupled with precipitation-dissolution reaction models).

The paper is structured as follows. We begin with a brief description of the model in Section 2 followed by Section 3 which deals with the notations used in this work. We proceed to define the mixed variational formulation in Section 4 where we prove the uniqueness of the solution with the existence coming from the convergence proof. Next, in sections 5 and 6 the time-discrete, respectively fully discrete numerical schemes are considered and the proofs for the convergence are provided. The numerical experiments are shown in Section 7 followed by the conclusions and discussions in Section 8.

2. The mathematical model. We consider a Darcy scale model that describes the reactive transport of the ions/solutes in a porous medium. The solutes are subjected to convective transport and in addition they undergo diffusion and reactions in the bulk. Below we provide a brief description and the assumptions of the model; we refer to [15], or [16] for more details.

Let  $\Omega \subset \mathbb{R}^2$  be the domain occupied by the porous medium, and assume  $\Omega$  be open, connected, bounded and with Lipschitz boundary  $\Gamma$ . Further, let T > 0 be a fixed but arbitrarily chosen time, and define

$$\Omega^T = (0, T] \times \Omega$$
, and  $\Gamma^T = (0, T] \times \Gamma$ .

At the outset, we assume that the fluid velocity  $\mathbf{q}$  is known, divergence free and essentially bounded

$$\nabla \cdot \mathbf{q} = 0$$
 in  $\Omega$ .

Usually, two or more different types of ions react to produce precipitate (an immobile species). A simplified model will be considered here where we include only one mobile species. This makes

#### Numerical Analysis

sense if the boundary and initial data are compatible (see [15], or [16]). Then, denoting by v the concentration of the (immobile) precipitate, and by u the cation concentration, the model reduces to

$$\begin{cases} \partial_t (u+v) + \nabla \cdot (\mathbf{q}u - \nabla u) &= 0, \quad \text{in } \Omega^T, \\ u &= 0, \quad \text{on } \Gamma^T, \\ u &= u_I, \quad \text{in } \Omega, \text{ for } t = 0, \end{cases}$$
(2.1)

for the ion transport, and

$$\begin{cases} \partial_t v &= (r(u) - w), \quad \text{on } \Omega^T, \\ w &\in H(v), \quad \text{on } \Omega^T, \\ v &= v_I, \quad \text{on } \Omega, \text{ for } t = 0, \end{cases}$$

$$(2.2)$$

for the precipitate. For the ease of presentation we restrict to homogeneous Dirichlet boundary conditions. The assumptions for the initial conditions will be given below. In the system considered above, we assume all the quantities and variables as dimensionless. To simplify the exposition, the diffusion is assumed 1, the extension to a positive definite diffusion tensor being straightforward. Further, we assume that the Damköhler number is scaled to 1, as well as an eventual factor in the time derivative of v in  $(2.2)_1$ , appearing in the transition form the pore scale to the core scale.

The assumptions on the precipitation rate r are (A.r1)  $r(\cdot) : \mathbb{R} \to [0, \infty)$  is Lipschitz in  $\mathbb{R}$  with the constant  $L_r$ . (A.r2) There exists a unique  $u_* \ge 0$ , such that

$$r(u) = \begin{cases} 0 \text{ for } u \leq u_*, \\ \text{strictly increasing for } u \geq u_* \text{ with } r(\infty) = \infty. \end{cases}$$
(2.3)

The interesting part is the structure of the dissolution rate. We interpret it as a process encountered strictly at the surface of the precipitate layer, so the rate is assumed constant (1, by scaling) at some  $(t, x) \in \Omega^T$  where the precipitate is present, i.e. if v(t, x) > 0. In the absence of the precipitate, the overall rate (precipitate minus dissolution) is either zero, if the solute present there is insufficient to produce a net precipitation gain, or positive. This can be summarized as

$$w \in H(v), \quad \text{where} \quad H(v) = \begin{cases} 0, & \text{if } v < 0, \\ [0,1] & \text{if } v = 0, \\ 1 & \text{if } v > 0. \end{cases}$$
(2.4)

In the setting above, a unique  $u^*$  exists for which  $r(u^*) = 1$ . If  $u = u^*$  for all t and x, then the system is in equilibrium: no precipitation or dissolution occurs, since the precipitation rate is balanced by the dissolution rate regardless of the presence of absence of crystals (see [26], Section 5 for some illustrations). Then, as follows from [23, 18, 31], for a.e.  $(t, x) \in \Omega^T$  where v = 0, the dissolution rate satisfies

$$w = \begin{cases} r(u) & \text{if } u < u^*, \\ 1 & \text{if } u \ge u^*. \end{cases}$$
(2.5)

Since, we will work with the model in the mixed formulation, we define the flux as

$$\mathbf{Q} = -\nabla u + \mathbf{q}u. \tag{2.6}$$

Except for some particular situations, one cannot expect the existence of classical solutions to (2.1)-(2.2). To rectify this, we resort to defining appropriate weak solutions which implies satisfying the equations in some average sense. Formally, these solutions are obtained by multiplying by smooth functions and using partial integration wherever required thereby reducing the regularity of solutions otherwise needed in the strong form. In this work, we write the equations in a mixed variational form which means that we separate the equation for the flux  $\mathbf{Q}$  and retain the local mass conservation property (see [36, 37, 38] for similar problems).

Kumar, Pop, and Radu

**3.** Notations. We adopt the following notations from the functional analysis. In particular, by  $H_0^1(\Omega)$  we mean the space of functions in  $H^1(\Omega)$  and having a vanishing trace on  $\Gamma$  and  $H^{-1}$  is its dual. By  $(\cdot, \cdot)$  we mean  $L^2$  inner product or the duality pairing between  $H_0^1$  and  $H^{-1}$ . Further,  $\|\cdot\|$  stands for the norms induced by  $L^2$  inner product. For other norms, we explicitly state it. The functions in  $H(div; \Omega)$  are vector valued having a  $L^2$  divergence. Furthermore, C denotes a generic constant and the value of which might change from line to line and is independent of unknown variables or the discretization parameters.

Having introduced these notations we can state the assumptions on the initial conditions:

(A.I1) The initial data  $u_I$  and  $v_I$  are non-negative and essentially bounded.

(A.I2)  $u_I, v_I \in H^1_0(\Omega)$ .

We have taken the initial conditions in  $H_0^1$  to avoid technicalities. Alternatively, one can approximate the initial conditions by taking the convolutions with smooth functions. The  $H_0^1$  regularity for  $v_I$  is used for obtaining strong convergence results, for which  $L^2$  regularity is not sufficient.

We furthermore assume that  $\Omega$  is polygonal. Therefore it admits regular decompositions into simplices and the errors due to nonpolygonal domains are avoided. The spatial discretization will be defined on such a regular decomposition  $\mathcal{T}_h$  into 2D simplices (triangles); h stands for the mesh-size. We provide the exposition for 2D but extending the results to 3D is similar.

We define the following sets

$$\begin{aligned} \mathcal{V} &:= \{ v \in H^1((0,T); L^2(\Omega)) \}, \\ \mathcal{S} &:= \{ \mathbf{Q} \mid \mathbf{Q} \in L^2((0,T); H(div; \Omega)) \}, \\ \mathcal{W} &:= \{ w \in L^{\infty}(\Omega^T), : 0 \le w \le 1 \}. \end{aligned}$$

In addition, for the fully discrete situation, we use the following discrete subspaces  $\mathcal{V}_h \subset L^2(\Omega)$ and  $\mathcal{S}_h \subset H(div; \Omega)$  defined as follows

$$\mathcal{V}_h := \{ u \in L^2(\Omega) \mid u \text{ is constant on each element } T \in \mathcal{T}_h \}$$
  
$$\mathcal{S}_h := \{ \mathbf{Q} \in H(\operatorname{div}; \Omega) \mid \mathbf{Q}_{|_T} = \mathbf{a} + b\mathbf{x} \text{ for all } T \in \mathcal{T}_h \}.$$

In other words,  $\mathcal{V}_h$  denotes the space of piecewise constant functions, while  $\mathcal{S}_h$  is the  $RT_0$  space. Clearly from the above definitions,  $\nabla \cdot \mathbf{Q} \in \mathcal{V}_h$  for any  $\mathbf{Q} \in \mathcal{S}_h$ .

We also define the following usual projections:

$$P_h: L^2(\Omega) \mapsto \mathcal{V}_h, \langle P_h v - v, v_h \rangle = 0$$

for all  $v_h \in \mathcal{V}_h$ . Similarly, the projection  $\Pi_h$  is defined on  $(H^1(\Omega))^d$  such that

$$\Pi_h : (H^1(\Omega))^d \mapsto \mathcal{S}_h, \langle \nabla \cdot (\Pi_h \mathbf{Q} - \mathbf{Q}), v_h \rangle = 0$$

for all  $v_h \in \mathcal{V}_h$ . Following [35], p.237 (also see [9]), this operator can be extended to  $H(div; \Omega)$  and also for the above operators there holds

$$\|v - P_h v\| \le Ch \|v\|_{H^1(\Omega)} \tag{3.1}$$

and further,

$$\|\mathbf{Q} - \Pi_{h}\mathbf{Q}\| \leq Ch\|\mathbf{Q}\|_{H^{1}(\Omega)}$$
  
$$\|\nabla \cdot \mathbf{Q} - \nabla \cdot (\Pi_{h}\mathbf{Q})\| \leq Ch\|\mathbf{Q}\|_{H^{2}(\Omega)}.$$
  
(3.2)

For the spatial discretization we will work with the approximation  $\mathbf{q}_h$  of the Darcy velocity  $\mathbf{q}$ ,

defined on the given mesh  $\mathcal{T}_h$ . For this approximation we assume that there exists a  $M_q > 0$  s.t.  $\|\mathbf{q}_h\|_{L^{\infty}} \leq M_q$  (uniformly in h; the same estimate being valid for  $\mathbf{q}$ ), and as  $h \searrow 0$ 

$$\|\mathbf{q}_h - \mathbf{q}\|_{L^2(\Omega)^2} \to 0. \tag{3.3}$$

Having stated the assumptions, we proceed by introducing the mixed variational formulation and analyzing the convergence of its discretization.

4. Continuous mixed variational formulation. A weak solution of (2.1)-(2.2) written in mixed form is defined as follows.

DEFINITION 4.1. A quadruple  $(u, \mathbf{Q}, v, w) \in (\mathcal{V} \times \mathcal{S} \times \mathcal{V} \times \mathcal{W} \text{ with } u_{|t=0} = u_I, v_{|t=0} = v_I$ is a mixed weak solution of (2.1)-(2.2) if  $w \in H(v)$  a.e. and for all  $t \in (0,T)$  and  $(\phi, \theta, \psi) \in H^1(\Omega) \times L^2(\Omega) \times H(div; \Omega)$  we have

$$\begin{aligned} (\partial_t u, \phi) + (\nabla \cdot \boldsymbol{Q}, \phi) + (\partial_t v, \phi) &= 0, \\ (\partial_t v, \theta) - (r(u) - w, \theta) &= 0, \\ (\boldsymbol{Q}, \boldsymbol{\psi}) - (u, \nabla \cdot \boldsymbol{\psi}) - (\boldsymbol{q} u, \boldsymbol{\psi}) &= 0. \end{aligned}$$

$$(4.1)$$

The proof for the existence of solution for (4.1) is obtained by the convergence of the numerical schemes considered below. Therefore, we give the proof for the uniqueness of the solution. The following lemma shows the uniqueness without further details on w. As mentioned in (2.5) the inclusion  $w \in H(v)$  can be made more precise.

LEMMA 4.2. The mixed weak formulation (4.1) has at most one solution.

*Proof.* Assume there exist two solution quadruples  $(u_1, \mathbf{Q}_1, v_1, w_1)$  and  $(u_2, \mathbf{Q}_2, v_2, w_2)$ , and define

$$u := u_1 - u_2$$
,  $\mathbf{Q} := \mathbf{Q}_1 - \mathbf{Q}_2$ ,  $v := v_1 - v_2$ ,  $w := w_1 - w_2$ .

Clearly, at t = 0 we have u(0, x) = 0 and v(0, x) = 0 for all x. Subtracting (4.1)<sub>2</sub> for  $u_2, v_2$  and  $w_2$  from the equation for  $u_1, v_1$  and  $w_1$  and taking (for  $t \leq T$  arbitrary)  $\theta = \chi_{(0,t)}v$ , using monotonicity of H and the Lipschitz continuity of  $r(\cdot)$  leads to

$$\begin{aligned} \|v(t,\cdot)\|^2 &= \int_0^t \int_\Omega (r(u_1) - r(u_2))v(s,x)dxds - \int_0^t \int_\Omega (H(v_1) - H(v_2))v(s,x)dxds \\ &\leq \frac{1}{2} \int_0^t L_r^2 \|u(s,\cdot)\|^2 ds + \frac{1}{2} \int_0^t \|v(s,\cdot)\|^2 ds. \end{aligned}$$

Then Gronwall's lemma gives

$$\|v(t,\cdot)\|^{2} \leq Ce^{t} \int_{0}^{t} \|u(s,\cdot)\|^{2} ds \leq C \int_{0}^{t} \|u(s,\cdot)\|^{2} ds.$$
(4.2)

Next, we choose for  $\phi = \chi_{(0,t)} u(t,x)$  in the difference between the two equalities (4.1)<sub>1</sub> to get

$$\|u(t,\cdot)\|^2 + \left(\int_0^t \nabla \cdot \mathbf{Q}(s,\cdot)ds, u(t,\cdot)\right) + (v(t,\cdot), u(t,\cdot)) = 0.$$

$$(4.3)$$

Similarly, choosing  $\psi = \int_{0}^{t} \mathbf{Q}(s) ds$  in (4.1)<sub>3</sub> (written for a.e. t) yields

$$\int_{\Omega} \left( \mathbf{Q}(t,x) \int_{0}^{t} \mathbf{Q}(s,x) ds \right) dx - \int_{\Omega} u(t,x) \left( \int_{0}^{t} \nabla \cdot \mathbf{Q}(s,x) ds \right) dx - \int_{\Omega} \mathbf{q} u(t,x) \left( \int_{0}^{t} \mathbf{Q}(s,x) ds \right) dx = 0.$$
(4.4)

Combining (4.3) and (4.4) we have

$$\begin{split} \|u(t,\cdot)\|^2 + \int\limits_{\Omega} v(t,x)u(t,x)dx + \int\limits_{\Omega} \mathbf{Q}(t,x) \int\limits_{0}^{t} \mathbf{Q}(s,x)dsdx &= \int\limits_{\Omega} \mathbf{q}u(t,x) \int\limits_{0}^{t} \mathbf{Q}dsdx \\ &\leq \frac{1}{4} \|u(t,\cdot)\|^2 + M_q^2 \left\| \int\limits_{0}^{t} \mathbf{Q}(s,\cdot)ds \right\|^2, \end{split}$$

which implies,

$$\|u(t,\cdot)\|^{2} + (\mathbf{Q}(t,\cdot), \int_{0}^{t} \mathbf{Q}(s,\cdot)ds) \leq \frac{1}{2}\|u(t,\cdot)\|^{2} + M_{q}^{2} \left\|\int_{0}^{t} \mathbf{Q}ds\right\|^{2} + \|v(t,\cdot)\|^{2}.$$

Using (4.2) we obtain

$$\frac{1}{2} \|u(t,\cdot)\|^2 + (\mathbf{Q}(t,\cdot), \int_0^t \mathbf{Q}(s,\cdot)ds) \le C \int_0^t \|u(s,\cdot)\|^2 ds + M_q^2 \left\| \int_0^t \mathbf{Q}(s,\cdot)ds \right\|^2.$$
(4.5)

Defining,

$$E(t) := \frac{1}{2} \int_{0}^{t} \|u(s, \cdot)\|^{2} ds + \frac{1}{2} \left\| \int_{0}^{t} \mathbf{Q}(s) ds \right\|^{2}$$

we have  $E \ge 0$  and E(0) = 0 because of initial conditions. Then (4.5) rewrites

$$\frac{dE}{dt} \le CE.$$

This immediately gives E(t) = 0 for all t implying

$$\int_{0}^{t} \|u(s,\cdot)\|^{2} ds = 0, \text{ and } \int_{0}^{t} \mathbf{Q}(s) ds = 0$$

for all t. Hence  $u = 0, \mathbf{Q} = 0$  and using this in (4.2) we conclude v = 0.

#### Numerical Analysis

5. Semi-discrete mixed variational formulation. As announced, to avoid dealing with inclusion in the description of dissolution rate, the numerical scheme relies on the regularization of the Heaviside graph. With this aim, with  $\delta > 0$  we define

$$H_{\delta}(z) := \begin{cases} 1, & z > \delta, \\ \frac{z}{\delta}, & 0 \le z \le \delta, \\ 0, & z < 0. \end{cases}$$
(5.1)

Next, with  $N \in \mathbb{N}, \tau = \frac{T}{N}$  and  $t_n = n\tau, n = 1, \dots, N$ , we consider a first order time discretization with uniform time stepping, which is implicit in u and explicit in v. At each time stepping to a whith anisother time stepping, which is implicit in a tail explicit in  $\mathfrak{C}$ . It can time stepping  $t_n$  we use  $(u_{\delta}^{n-1}, v_{\delta}^{n-1}) \in (L^2(\Omega), L^2(\Omega))$  detemined at  $t_{n-1}$  to find the next approximation  $(u_{\delta}^n, \mathbf{Q}_{\delta}^n, v_{\delta}^n, \mathbf{w}^n)$ . The procedure is initiated with  $u^0 = u_I, v^0 = v_I$ . Specifically, we look for  $(u_{\delta}^n, v_{\delta}^n, \mathbf{Q}_{\delta}^n) \in H^1(\Omega), L^2(\Omega), H(div; \Omega)$  satisfying the time discrete

 $\mathbf{Problem} \ \mathbf{P}_{\delta}^{mvf,n} \text{: } \text{Given } (u_{\delta}^{n-1}, v_{\delta}^{n-1}) \in \left(L^{2}(\Omega), L^{2}(\Omega)\right), \text{ find } (u_{\delta}^{n}, \mathbf{Q}_{\delta}^{n}, v_{\delta}^{n}, w_{\delta}^{n}) \in \left(L^{2}(\Omega), H(div; \Omega), (u_{\delta}^{n-1}, v_{\delta}^{n-1})\right)$  $L^2(\Omega), L^{\infty}(\Omega)$  such that

$$\begin{aligned} & (u_{\delta}^{n} - u_{\delta}^{n-1}, \phi) + \tau(\nabla \cdot \mathbf{Q}_{\delta}^{n}, \phi) + (v_{\delta}^{n} - v_{\delta}^{n-1}, \phi) = 0, \\ & (v_{\delta}^{n} - v_{\delta}^{n-1}, \theta) - \tau(r(u_{\delta}^{n}), \theta) - \tau(H_{\delta}(v_{\delta}^{n-1}), \theta) = 0, \\ & (\mathbf{Q}_{\delta}^{n}, \psi) - (u_{\delta}^{n}, \nabla \cdot \psi) - (\mathbf{q}u_{\delta}^{n}, \psi) = 0 \end{aligned}$$
(5.2)

for all  $(\phi, \theta, \psi) \in (H^1(\Omega), L^2(\Omega), H(div; \Omega))$ . For completeness we define

$$w^n_{\delta} = H_{\delta}(v^n_{\delta}).$$

This is a system of elliptic equations for  $u_{\delta}^{n}, \mathbf{Q}_{\delta}^{n}, v_{\delta}^{n}$  given  $u_{\delta}^{n-1} \in H^{1}_{0,\Gamma_{D}}(\Omega), v_{\delta}^{n-1} \in L^{2}(\Omega)$ . For stability reasons, we choose  $\delta = O(\tau^{\frac{1}{2}})$  (see [14, 26] for detailed arguments) which implies that  $\frac{\tau}{\delta}$  goes to 0 as  $\tau \searrow 0$ . This in turn allows us to consider the solutions along the sequence of regularized Heaviside function with the regularization parameter  $\delta$  automatically vanishing in the limit of  $\tau \searrow 0$ .

The existence of a solution for Problem  $\mathbf{P}_{\delta}^{mvf,n}$  will result from the convergence of the fully discrete scheme, which is proved in the Appendix by keeping  $\tau$  and  $\delta$  fixed, and passing to the limit  $h \searrow 0$ . Note that it suffices to compute  $u_{\delta}^n$ , as  $v_{\delta}^n$  can be obtained straightforwardly. For now, we prove the uniqueness of the solution. LEMMA 5.1. Problem  $\boldsymbol{P}_{\delta}^{mvf,n}$  has at most one solution triple  $(u_{\delta}^{n}, \boldsymbol{Q}_{\delta}^{n}, v_{\delta}^{n})$ .

*Proof.* Since  $w_{\delta}^n = H_{\delta}(v_{\delta}^n)$ , it has no influence on the existence or uniqueness of the solution. Therefore, we consider only the triples  $(u_{\delta}^n, \mathbf{Q}_{\delta}^n, v_{\delta}^n)$ . Assume that for the same  $(u_{\delta}^{n-1}, v_{\delta}^{n-1})$  there are two solution triples  $(u_{\delta,i}^n, \mathbf{Q}_{\delta,i}^n, v_{\delta,i}^n)$ , i = 1, 2 providing a solution to Problem  $\mathbf{P}_{\delta}^{mvf,n}$ . Define

$$u_{\delta}^n := u_{\delta,1}^n - u_{\delta,2}^n, \quad \mathbf{Q}_{\delta}^n := \mathbf{Q}_{\delta,1}^n - \mathbf{Q}_{\delta,2}^n, \quad v_{\delta}^n := v_{\delta,1}^n - v_{\delta,2}^n$$

We follow the usual approach and consider the equations for the difference above. Taking  $\theta = v_{\delta}^{n}$ in  $(5.2)_2$  gives

$$\|v_{\delta}^{n}\|^{2} = \tau(r(u_{\delta,1}^{n}) - r(u_{\delta,2}^{n}), v_{\delta}^{n}) \le \tau L_{r} \|u_{\delta}^{n}\| \|v_{\delta}^{n}\|$$

as the  $H_{\delta}$  terms cancel because of explicit discretization. This gives,

$$\|v_{\delta}^n\| \le C\tau \|u_{\delta}^n\|. \tag{5.3}$$

Further, with  $\phi = u_{\delta}^{n}, \theta = u_{\delta}^{n}, \psi = \tau \mathbf{Q}_{\delta}^{n}$ , from (5.2) we obtain

$$\|u_{\delta}^n\|^2 + \tau \|\mathbf{Q}_{\delta}^n\|^2 + \tau (r(u_{\delta,1}^n) - r(u_{\delta,2}^n), u_{\delta}^n) = \tau (\mathbf{q}u_{\delta}^n, \mathbf{Q}_{\delta}^n).$$

Since r is monotone, the Cauchy inequality and boundedness of  $\mathbf{q}$  give

$$||u_{\delta}^{n}||^{2} + \frac{1}{2}\tau ||\mathbf{Q}_{\delta}^{n}||^{2} \le \tau \frac{1}{2}M_{q}^{2}||u_{\delta}^{n}||^{2}.$$

For  $\tau < \frac{2}{M_q^2}$ , we obtain

$$||u_{\delta}^{n}|| = 0$$
 and thereby  $||\mathbf{Q}_{\delta}^{n}|| = 0$ .

Together with (5.3) we conclude  $u_{\delta}^{n} = v_{\delta}^{n} = 0$  and  $\mathbf{Q}_{\delta}^{n} = \mathbf{0}$ .  $\Box$ 

5.1. The a priori estimates. We start with the following stability estimates.

LEMMA 5.2. It holds that

$$\sup_{k=1,\dots,N} \left\| u_{\delta}^k \right\| \le C \tag{5.4}$$

$$\left\| v_{\delta}^{n} - v_{\delta}^{n-1} \right\| \le C\tau \tag{5.5}$$

$$\sup_{k=1,\dots,N} \|v_{\delta}^{\kappa}\| \le C \tag{5.6}$$

$$\sup_{k=1,\dots,N} \left\| \boldsymbol{Q}_{\delta}^k \right\| \le C \tag{5.7}$$

$$\sum_{n=1}^{N} \left\| u_{\delta}^{n} - u_{\delta}^{n-1} \right\|^{2} \le C\tau$$
(5.8)

$$\sum_{n=1}^{N} \left\| \boldsymbol{Q}_{\delta}^{n} - \boldsymbol{Q}_{\delta}^{n-1} \right\|^{2} \le C$$
(5.9)

$$\sum_{n=1}^{N} \tau \left\| \nabla \cdot \boldsymbol{Q}_{\delta}^{n} \right\|^{2} \le C$$
(5.10)

$$\sum_{n=1}^{N} \tau \left\| \nabla \cdot \left( \boldsymbol{Q}_{\delta}^{n} - \boldsymbol{Q}_{\delta}^{n-1} \right) \right\|^{2} \leq C.$$
(5.11)

*Proof.* We start by showing (5.4). To this aim we chose

$$\phi = u_{\delta}^n, \quad \psi = \tau \mathbf{Q}_{\delta}^n, \quad \theta = u_{\delta}^n$$

as test functions in (5.2), and add the resulting to obtain

$$(u_{\delta}^{n} - u_{\delta}^{n-1}, u_{\delta}^{n}) + \tau \left\|\mathbf{Q}_{\delta}^{n}\right\|^{2} - \tau(\mathbf{q}u_{\delta}^{n}, \mathbf{Q}_{\delta}^{n}) + \tau(r(u_{\delta}^{n}), u_{\delta}^{n}) = \tau(H_{\delta}(v_{\delta}^{n-1}), u_{\delta}^{n}).$$
(5.12)

Using the equality

$$(u_{\delta}^{n} - u_{\delta}^{n-1}, u_{\delta}^{n}) = \frac{1}{2} \left( \|u_{\delta}^{n}\|^{2} - \|u_{\delta}^{n-1}\|^{2} + \|u_{\delta}^{n} - u_{\delta}^{n-1}\|^{2} \right)$$

since **q** and  $H_{\delta}$  are bounded and  $r(u_{\delta}^n)u_{\delta}^n \ge 0$ , by Young's inequality we get

$$\|u_{\delta}^{n}\|^{2} - \|u_{\delta}^{n-1}\|^{2} + \|u_{\delta}^{n} - u_{\delta}^{n-1}\|^{2} + 2\tau \|\mathbf{Q}_{\delta}^{n}\|^{2} + 2\tau(r(u_{\delta}^{n}), u_{\delta}^{n})$$
  
=  $2\tau(\mathbf{q}u_{\delta}^{n}, \mathbf{Q}_{\delta}^{n}) + 2\tau(H_{\delta}(v_{\delta}^{n-1}), u_{\delta}^{n}) \leq \tau \|\mathbf{Q}_{\delta}^{n}\|^{2} + C\tau \|u_{\delta}^{n}\|^{2} + C\tau + C\tau \|u_{\delta}^{n}\|^{2}.$ 

Summing over n = 1, ..., k (where  $k \in \{1, ..., N\}$  is arbitrary) gives

$$\left\|u_{\delta}^{k}\right\|^{2} + \sum_{n=1}^{k} \left\|u_{\delta}^{n} - u_{\delta}^{n-1}\right\|^{2} + \tau \sum_{n=1}^{k} \left\|\mathbf{Q}_{\delta}^{n}\right\|^{2} \le \left\|u_{I}\right\|^{2} + C + C\tau \sum_{n=1}^{k} \left\|u_{\delta}^{n}\right\|^{2},$$
(5.13)

and (5.4) follows from the discrete Gronwall lemma.

For (5.5) we choose for  $\theta = v_{\delta}^n - v_{\delta}^{n-1}$  in (5.2)<sub>2</sub> and apply the Cauchy Schwarz inequality for the right hand side,

$$\left\| v_{\delta}^{n} - v_{\delta}^{n-1} \right\|^{2} \leq \tau \left\| r(u_{\delta}^{n}) \right\| \left\| v_{\delta}^{n} - v_{\delta}^{n-1} \right\| + \tau \left\| H_{\delta}(v_{\delta}^{n-1}) \right\| \left\| v_{\delta}^{n} - v_{\delta}^{n-1} \right\|.$$

Using (5.4), the boundedness of  $H_{\delta}$  and the Lipschitz continuity of r this implies

$$\left\| v_{\delta}^{n} - v_{\delta}^{n-1} \right\| \le C\tau.$$

To prove (5.6), choose  $\theta = v_{\delta}^n$  in (5.2)<sub>2</sub> to obtain

$$(v_{\delta}^n - v_{\delta}^{n-1}, v_{\delta}^n) = \tau(r(u_{\delta}^n), v_{\delta}^n) - \tau(H_{\delta}(v_{\delta}^{n-1}), v_{\delta}^n).$$

The left hand side can be rewritten as

$$(v_{\delta}^{n} - v_{\delta}^{n-1}, v_{\delta}^{n}) = \frac{1}{2} \left( \|v_{\delta}^{n}\|^{2} - \|v_{\delta}^{n-1}\|^{2} + \|v_{\delta}^{n} - v_{\delta}^{n-1}\|^{2} \right).$$

We write the last term on the right hand side as

$$\left(H_{\delta}(v_{\delta}^{n-1}), v_{\delta}^{n}\right) = \left(H_{\delta}(v_{\delta}^{n-1}), v_{\delta}^{n-1}\right) - \left(H_{\delta}(v_{\delta}^{n-1}), v_{\delta}^{n-1} - v_{\delta}^{n}\right).$$

and substitute it in above to obtain

$$\|v_{\delta}^{n}\|^{2} - \|v_{\delta}^{n-1}\|^{2} + \|v_{\delta}^{n} - v_{\delta}^{n-1}\|^{2} = 2\tau \left(r(u_{\delta}^{n}), v_{\delta}^{n}\right) - \left(H_{\delta}(v_{\delta}^{n-1}), v_{\delta}^{n-1}\right) + \left(H_{\delta}(v_{\delta}^{n-1}), v_{\delta}^{n-1} - v_{\delta}^{n}\right).$$
  
Since  $H(\cdot)$  is monotone,  $(H_{\delta}(v_{\delta}^{n-1}), v_{\delta}^{n-1}) \ge 0$ , now the Cauchy Schwarz inequality gives

the 
$$\Pi(\cdot)$$
 is monotone,  $(\Pi_{\delta}(v_{\delta}), v_{\delta}) \geq 0$ , now the Cauchy Schwarz mequality gives

$$\|v_{\delta}^{n}\|^{2} - \|v_{\delta}^{n-1}\|^{2} + \|v_{\delta}^{n} - v_{\delta}^{n-1}\|^{2} \le 2\tau C \|u_{\delta}^{n}\| \|v_{\delta}^{n}\| + 2\tau \left(H_{\delta}(v_{\delta}^{n-1}), v_{\delta}^{n} - v_{\delta}^{n-1}\right).$$

By Young's inequality this leads to

$$\|v_{\delta}^{n}\|^{2} - \|v_{\delta}^{n-1}\|^{2} + \frac{1}{2} \|v_{\delta}^{n} - v_{\delta}^{n-1}\|^{2} \le \tau \|v_{\delta}^{n}\|^{2} + C\tau \|u_{\delta}^{n}\|^{2} + 2\tau^{2} \|H_{\delta}\|^{2}.$$

Summing over n = 1, ..., k (with  $k \in \{1, ..., N\}$  arbitrary) this gives

$$\begin{aligned} \left\| v_{\delta}^{k} \right\|^{2} + \sum_{n=1}^{k} \left\| v_{\delta}^{n} - v_{\delta}^{n-1} \right\|^{2} &\leq \| v_{I} \|^{2} + \tau \sum_{n=1}^{k} \| v_{\delta}^{n} \|^{2} + C\tau \sum_{n=1}^{k} \| u_{\delta}^{n} \|^{2} + \sum_{n=1}^{k} 4\tau^{2} \| H_{\delta} \|^{2} \\ &\leq \tau \sum_{n=1}^{k} \| v_{\delta}^{n} \|^{2} + C + C\tau \end{aligned}$$

where we have used the estimates proved before and the bounds on initial data. Now (5.6) follows from the Discrete Gronwall Lemma.

We proceed with the estimate (5.7). To this aim, we need to specify the initial flux:  $\mathbf{Q}^0_{\delta} = -\nabla u_I + \mathbf{q} u_I \in (L^2(\Omega))^d$ . With  $\phi = u^n_{\delta} - u^{n-1}_{\delta}$ , (5.2)<sub>1</sub> gives

$$\left\|u_{\delta}^{n}-u_{\delta}^{n-1}\right\|^{2}+\tau\left(\nabla\cdot\mathbf{Q}_{\delta}^{n},u_{\delta}^{n}-u_{\delta}^{n-1}\right)+\left(v_{\delta}^{n}-v_{\delta}^{n-1},u_{\delta}^{n}-u_{\delta}^{n-1}\right)=0.$$
(5.14)

Now take  $\boldsymbol{\psi} = \tau \mathbf{Q}_{\delta}^{n}$  to get

$$\tau \left(\mathbf{Q}^{n}_{\delta}, \mathbf{Q}^{n}_{\delta}\right) - \tau \left(u^{n}_{\delta}, \nabla \cdot \mathbf{Q}^{n}_{\delta}\right) - \tau \left(\mathbf{q}u^{n}_{\delta}, \mathbf{Q}^{n}_{\delta}\right) = 0, \tag{5.15}$$

and next choose  $\boldsymbol{\psi}=\tau\mathbf{Q}_{\delta}^{n}$  for the equation corresponding to (n-1)-th time step

$$\tau\left(\mathbf{Q}_{\delta}^{n-1},\mathbf{Q}_{\delta}^{n}\right)-\tau\left(u_{\delta}^{n-1},\nabla\cdot\mathbf{Q}_{\delta}^{n}\right)-\tau\left(\mathbf{q}u_{\delta}^{n-1},\mathbf{Q}_{\delta}^{n}\right)=0.$$
(5.16)

Subtract (5.16) from (5.15) to obtain

$$\tau \left( \mathbf{Q}_{\delta}^{n} - \mathbf{Q}_{\delta}^{n-1}, \mathbf{Q}_{\delta}^{n} \right) - \tau \left( u_{\delta}^{n} - u_{\delta}^{n-1}, \nabla \cdot \mathbf{Q}_{\delta}^{n} \right) - \tau \left( \mathbf{q}(u_{\delta}^{n} - u_{\delta}^{n-1}), \mathbf{Q}_{\delta}^{n} \right) = 0$$

Further, use (5.14) in above to obtain

$$\left\|u_{\delta}^{n}-u_{\delta}^{n-1}\right\|^{2}+\tau\left(\mathbf{Q}_{\delta}^{n}-\mathbf{Q}_{\delta}^{n-1},\mathbf{Q}_{\delta}^{n}\right)=\tau\left(\mathbf{q}(u_{\delta}^{n}-u_{\delta}^{n-1}),\mathbf{Q}_{\delta}^{n}\right)-(v_{\delta}^{n}-v_{\delta}^{n-1},u_{\delta}^{n}-u_{\delta}^{n-1}).$$
 (5.17)  
s before, we can rewrite  $(\mathbf{Q}_{\delta}^{n}-\mathbf{Q}_{\delta}^{n-1},\mathbf{Q}_{\delta}^{n})$  as

As  $\mathbf{z}_{\delta}$  $(\mathbf{v}_{\delta})$  $, \mathbf{v}_{\delta})$ 

$$\left(\mathbf{Q}_{\delta}^{n}-\mathbf{Q}_{\delta}^{n-1},\mathbf{Q}_{\delta}^{n}\right)=\frac{1}{2}\left(\|\mathbf{Q}_{\delta}^{n}\|^{2}-\|\mathbf{Q}_{\delta}^{n-1}\|^{2}+\|\mathbf{Q}_{\delta}^{n}-\mathbf{Q}_{\delta}^{n-1}\|^{2}\right).$$

Substituting the above in (5.17) we obtain

$$2 \| u_{\delta}^{n} - u_{\delta}^{n-1} \|^{2} + \tau \| \mathbf{Q}_{\delta}^{n} \|^{2} - \tau \| \mathbf{Q}_{\delta}^{n-1} \|^{2} + \tau \| \mathbf{Q}_{\delta}^{n} - \mathbf{Q}_{\delta}^{n-1} \|^{2} \\= 2\tau (\mathbf{q}(u_{\delta}^{n} - u_{\delta}^{n-1}), \mathbf{Q}_{\delta}^{n}) - 2(v_{\delta}^{n} - v_{\delta}^{n-1}, u_{\delta}^{n} - u_{\delta}^{n-1})$$

The right hand side can be estimated using Young's inequality in a straightforward manner

$$2 \left\| u_{\delta}^{n} - u_{\delta}^{n-1} \right\|^{2} + \tau \left\| \mathbf{Q}_{\delta}^{n} \right\|^{2} - \tau \left\| \mathbf{Q}_{\delta}^{n-1} \right\|^{2} + \tau \left\| \mathbf{Q}_{\delta}^{n} - \mathbf{Q}_{\delta}^{n-1} \right\|^{2} \\ \leq \left\| u_{\delta}^{n} - u_{\delta}^{n-1} \right\|^{2} + 2M_{q}^{2}\tau^{2} \left\| \mathbf{Q}_{\delta}^{n} \right\|^{2} + 2 \left\| v_{\delta}^{n} - v_{\delta}^{n-1} \right\|^{2}.$$

Summing over n = 1, ..., k ( $k \in \{1, ..., N\}$  arbitrary) we obtain

$$\sum_{n=1}^{k} \left\| u_{\delta}^{n} - u_{\delta}^{n-1} \right\|^{2} + \tau \left\| \mathbf{Q}_{\delta}^{k} \right\|^{2} + \tau \sum_{n=1}^{k} \left\| \mathbf{Q}_{\delta}^{n} - \mathbf{Q}_{\delta}^{n-1} \right\|^{2} \le C\tau + C\tau^{2} \sum_{n=1}^{k} \left\| \mathbf{Q}_{\delta}^{n} \right\|^{2} + \tau \left\| \mathbf{Q}_{I} \right\|^{2}.$$
(5.18)

The estimate (5.7) follows now by the Discrete Gronwall lemma. Moreover, from (5.18) we also get (5.8) and (5.9).

Finally, to prove (5.10) we take  $\phi = \nabla \cdot \mathbf{Q}_{\delta}^{n}$  in (5.2)<sub>1</sub> and use Young's inequality for the right hand side to obtain

$$\tau^{2} \|\nabla \cdot \mathbf{Q}_{\delta}^{n}\|^{2} \leq \left\|u_{\delta}^{n} - u_{\delta}^{n-1}\right\|^{2} + \left\|v_{\delta}^{n} - v_{\delta}^{n-1}\right\|^{2} + \frac{1}{2}\tau^{2} \|\nabla \cdot \mathbf{Q}_{\delta}^{n}\|^{2}.$$

Summing over n = 1..., N and using (5.5) and (5.8) gives (5.10).

Finally, to prove the estimate (5.11), we simply use the triangle inequality in (5.10).

5.2. Enhanced compactness. As will be seen below, the above estimates are not sufficient to retrieve the desired limiting equations. To complete the proof of convergence, stronger compactness properties are needed. These are obtained by translation estimates. To this aim, we define the translation in space

$$\Delta_{\xi} f(\cdot) := f(\cdot) - f(\cdot + \xi), \quad \xi \in \mathbb{R}^2.$$

Further, with  $\xi \in \mathbb{R}^2$  we consider  $\Omega_{\xi} \subset \Omega$  such that

$$\Omega_{\xi} := \{ x \in \Omega | \operatorname{dist}(\mathbf{x}, \Gamma) > \xi \}.$$

In this way, the translations  $\triangle_{\xi} f(x)$  with  $x \in \Omega$  are well-defined.

For reasons of brevity, the norms and the inner products for the translations should be understood with respect to  $\Omega_{\xi}$  unless explicitly stated otherwise. First, we consider the translation for  $u_{\delta}^{n}$ .

LEMMA 5.3. It holds that

$$\sum_{n=1}^{N} \tau \left\| \triangle_{\xi} u_{\delta}^{n} \right\|^{2} \le C |\xi|.$$

*Proof.* For  $(5.2)_3$  we have after translation in space

$$(\triangle_{\xi} \mathbf{Q}^{n}_{\delta}, \boldsymbol{\psi}) - (\triangle_{\xi} u^{n}_{\delta}, \nabla \cdot \boldsymbol{\psi}) - (\triangle_{\xi} (\mathbf{q} u^{n}_{\delta}), \boldsymbol{\psi}) = 0.$$

We construct an appropriate test function to obtain the estimate above. Take  $\eta^n$  such that

$$\begin{cases} -\Delta \eta^n = \triangle_{\xi} u^n_{\delta} & \text{in } \Omega \\ \eta^n = 0 & \text{on } \Gamma \end{cases}$$

and choose  $\psi = \nabla \eta^n$  (note that  $\psi \in H(div; \Omega)$ ) to obtain

$$(\triangle_{\xi} \mathbf{Q}^{n}_{\delta}, \nabla \eta^{n}) + (\triangle_{\xi} u^{n}_{\delta}, \triangle_{\xi} u^{n}_{\delta}) - (\triangle_{\xi} (\mathbf{q} u^{n}_{\delta}), \nabla \eta^{n}) = 0.$$
(5.19)

Note that  $\eta^n$  satisfies  $\| \bigtriangleup \eta^n \| = \| \bigtriangleup_{\xi} u^n_{\delta} \|$ , and therefore

$$\left\|\eta^{n}\right\|_{H^{2}(\Omega)} \leq C(\Omega) \left\|\bigtriangleup_{\xi} u_{\delta}^{n}\right\|$$

This implies that translations of  $\nabla \eta^n$  are controlled,

$$\left\|\nabla(\triangle_{\xi}\eta^{n})\right\|_{L^{2}(\Omega)} \leq C|\xi| \left\|\nabla\cdot(\nabla\eta^{n})\right\| \leq C(\Omega)|\xi| \left\|\triangle_{\xi}u_{\delta}^{n}\right\|.$$
(5.20)

Recalling (5.4), this gives

$$\|\nabla(\triangle_{\xi}\eta^{n})\|_{L^{2}(\Omega)} \leq C(\Omega)|\xi| \|\triangle_{\xi}u_{\delta}^{n}\| \leq C|\xi|.$$
(5.21)

Thus we have the following estimate

$$\tau \sum_{n=1}^{N} \left\| \bigtriangleup_{\xi} u_{\delta}^{n} \right\|^{2} = \tau \sum_{n=1}^{N} \left( \mathbf{q} u_{\delta}^{n}, \nabla(\bigtriangleup_{\xi} \eta^{n}) \right) + \tau \sum_{n=1}^{N} \left( \mathbf{Q}_{\delta}^{n}, \nabla(\bigtriangleup_{\xi} \eta^{n}) \right)$$

$$\leq \tau \sum_{n=1}^{N} \left\| \mathbf{Q}_{\delta}^{n} \right\| \left\| \nabla(\bigtriangleup_{\xi} \eta^{n}) \right\| + \tau \sum_{n=1}^{N} \left\| \mathbf{q} \right\|_{L^{\infty}(\Omega)} \left\| u_{\delta}^{n} \right\| \left\| \nabla(\bigtriangleup_{\xi} \eta^{n}) \right\|$$
(5.22)

The conclusion follows by (5.4), (5.7), the Young inequality and (5.21).  $\square$ 

The translation estimates for  $v_{\delta}^n$  are bounded by those for  $u_{\delta}^n$ . This is the essence of the next lemma.

LEMMA 5.4. The following estimates hold true

$$\sup_{k=1,\dots,N} \left\| \triangle_{\xi} v_{\delta}^{k} \right\|^{2} + \sum_{n=1}^{N} \left\| \triangle_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1}) \right\|^{2} \le C \left\| \triangle_{\xi} v_{I} \right\|^{2} + C\tau \sum_{n=1}^{N} \left\| \triangle_{\xi} u_{\delta}^{n} \right\|^{2}, \tag{5.23}$$

$$\sum_{n=1}^{N} \left\| \triangle_{\xi} v_{\delta}^{n} \right\|^{2} \le C |\xi|.$$
(5.24)

*Proof.* With  $\theta = \triangle_{\xi} v_{\delta}^n$  in  $(5.2)_2$ , we get

$$\left(\triangle_{\xi}v_{\delta}^{n}-\triangle_{\xi}v_{\delta}^{n-1},\triangle_{\xi}v_{\delta}^{n}\right)=\tau\left(\triangle_{\xi}r(u_{\delta}^{n}),\triangle_{\xi}v_{\delta}^{n}\right)-\tau\left(\triangle_{\xi}H_{\delta}(v_{\delta}^{n-1}),\triangle_{\xi}v_{\delta}^{n}\right)$$

The last term in the above rewrites as

$$\left(\triangle_{\xi}H_{\delta}(v_{\delta}^{n-1}),\triangle_{\xi}v_{\delta}^{n}\right) = \left(\triangle_{\xi}H_{\delta}(v_{\delta}^{n-1}),\triangle_{\xi}v_{\delta}^{n-1}\right) + \left(\triangle_{\xi}H_{\delta}(v_{\delta}^{n-1}),\triangle_{\xi}(v_{\delta}^{n}-v_{\delta}^{n-1})\right).$$

The monotonicity of  $H_{\delta}$  implies that the first term on the right hand side is positive

$$\left(\triangle_{\xi} H_{\delta}(v_{\delta}^{n-1}), \triangle_{\xi} v_{\delta}^{n-1}\right) \ge 0.$$

For the left hand side, we use the identity

$$\left(\triangle_{\xi}(v_{\delta}^{n}-v_{\delta}^{n-1}),\triangle_{\xi}v_{\delta}^{n}\right)=\frac{1}{2}\left(\left\|\triangle_{\xi}v_{\delta}^{n}\right\|^{2}-\left\|\triangle_{\xi}v_{\delta}^{n-1}\right\|^{2}+\left\|\triangle_{\xi}(v_{\delta}^{n}-v_{\delta}^{n-1})\right\|^{2}\right),$$

which, together with the Cauchy-Schwarz inequality for the first term on the right hand side gives

$$\frac{1}{2} \left( \left\| \bigtriangleup_{\xi} v_{\delta}^{n} \right\|^{2} - \left\| \bigtriangleup_{\xi} v_{\delta}^{n-1} \right\|^{2} + \left\| \bigtriangleup_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1}) \right\|^{2} \right) \\
\leq \tau L_{r} \left\| \bigtriangleup_{\xi} u_{\delta}^{n} \right\| \left\| \bigtriangleup_{\xi} v_{\delta}^{n} \right\| + \tau \left( \bigtriangleup_{\xi} H_{\delta} (v_{\delta}^{n-1}), \bigtriangleup_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1}) \right) \\
\leq L_{r} \frac{\tau}{2} \left\| \bigtriangleup_{\xi} u_{\delta}^{n} \right\|^{2} + \frac{\tau}{2} \left\| \bigtriangleup_{\xi} v_{\delta}^{n} \right\|^{2} + \tau^{2} \left\| \bigtriangleup_{\xi} H_{\delta} (v_{\delta}^{n-1}) \right\|^{2} + \frac{1}{4} \left\| \bigtriangleup_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1}) \right\|^{2} \\
\leq \frac{1}{2} L_{r} \tau \left\| \bigtriangleup_{\xi} u_{\delta}^{n} \right\|^{2} + \frac{1}{2} \tau \left\| \bigtriangleup_{\xi} v_{\delta}^{n} \right\|^{2} + \frac{\tau^{2}}{\delta^{2}} \left\| \bigtriangleup_{\xi} v_{\delta}^{n-1} \right\|^{2} + \frac{1}{4} \left\| \bigtriangleup_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1}) \right\|^{2}.$$

Summing over n = 1, ..., k  $(k \in \{1, ..., N\})$  yields

$$\begin{split} \left\| \triangle_{\xi} v_{\delta}^{k} \right\|^{2} &+ \frac{1}{2} \sum_{n=1}^{k} \left\| \triangle_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1}) \right\|^{2} \\ &\leq \left\| \triangle_{\xi} v_{I} \right\|^{2} + L_{r} \tau \sum_{n=1}^{k} \left\| \triangle_{\xi} u_{\delta}^{n} \right\|^{2} + \tau \sum_{n=1}^{k} \left\| \triangle_{\xi} v_{\delta}^{n} \right\|^{2} + \sum_{n=1}^{k} \frac{2\tau^{2}}{\delta^{2}} \left\| \triangle_{\xi} v_{\delta}^{n-1} \right\|^{2}. \end{split}$$
(5.25)

Using Lemma 5.3 and Gronwall's lemma we obtain

$$\sup_{k=1,...,N} \left\| \triangle_{\xi} v_{\delta}^{k} \right\|^{2} \le C\tau \sum_{n=1}^{N} \left\| \triangle_{\xi} u_{\delta}^{n} \right\|^{2} + \left\| \triangle_{\xi} v_{I} \right\|^{2}.$$
(5.26)

The estimate (5.23) follows from the above and from (5.25), whereas (5.24) is a direct consequence of Lemma 5.3 and the assumptions on  $v_I$ .  $\Box$ 

From the above we also get

LEMMA 5.5. The following estimate holds:

$$\sum_{n=1}^{N} \left\| \triangle_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1}) \right\| \le C\tau.$$
(5.27)

*Proof.* Testing in  $(5.2)_2$  with  $\theta = v_{\delta}^n - v_{\delta}^{n-1}$  gives

$$\begin{aligned} \left\| \triangle_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1}) \right\|^{2} &= \tau(\triangle_{\xi} r(u_{\delta}^{n}) - H_{\delta}(v_{\delta}^{n-1}), \triangle_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1})) \\ &\leq \tau^{2} \| \triangle_{\xi} r(u_{\delta}^{n}) \|^{2} + \frac{1}{2} \| \triangle_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1}) \|^{2} + \tau^{2} \| H_{\delta}(v_{\delta}^{n-1}) \|^{2}. \end{aligned}$$
(5.28)

Using the Lipschitz property of r and (5.4) we obtain

$$\left\| \bigtriangleup_{\xi} (v_{\delta}^{n} - v_{\delta}^{n-1}) \right\|^{2} \le \tau^{2} C,$$

and the conclusion follows by summing over  $n = 1, \dots, N$ .  $\Box$ 

**5.3.** Convergence. For proving the convergence of the time discretization scheme, we consider the sequence of time discrete quadruples  $\{(u_{\delta}^n, \mathbf{Q}_{\delta}^n, v_{\delta}^n, w_{\delta}^n), n = 0, \ldots, N\}$  solving Problem  $\mathbf{P}_{\delta}^{mvf,n}$ , and construct a time continuous approximation by linear interpolation. In this sense, for  $t \in [t_{n-1}, t_n]$   $(n = 1, \ldots, N)$  we define

$$U^{\tau}(t) := u_{\delta}^{n} \frac{(t - t_{n-1})}{\tau} + u_{\delta}^{n-1} \frac{(t_{n} - t)}{\tau},$$
  

$$V^{\tau}(t) := v_{\delta}^{n} \frac{(t - t_{n-1})}{\tau} + v_{\delta}^{n-1} \frac{(t_{n} - t)}{\tau},$$
  

$$\mathbf{Q}^{\tau}(t) := \mathbf{Q}_{\delta}^{n} \frac{(t - t_{n-1})}{\tau} + \mathbf{Q}_{\delta}^{n-1} \frac{(t_{n} - t)}{\tau},$$
  

$$W^{\tau}(t) := H_{\delta}(V^{\tau}(t)).$$
  
(5.29)

The estimates in Lemma 5.2 can be translated directly to  $(U^{\tau}, \mathbf{Q}^{\tau}, V^{\tau}, W^{\tau})$ :

LEMMA 5.6. A constant C > 0 exists s.t. for any  $\tau$  and  $\delta = O(\sqrt{\tau})$  the following  $L^2(0,T; L^2(\Omega))$  estimates hold

$$\|U^{\tau}\|^{2} + \|V^{\tau}\|^{2} + \|\boldsymbol{Q}^{\tau}\|^{2} \le C, \qquad (5.30)$$

$$\|\partial_t U^{\tau}\| + \|\partial_t V^{\tau}\|^2 + \|\nabla \cdot Q^{\tau}\|^2 \le C.$$
(5.31)

*Proof.* (5.30) follows easily from (5.4). For instance,

$$\|U^{\tau}\|^{2} \leq 2\|u_{\delta}^{n}\|^{2} + 2\|u_{\delta}^{n-1}\|^{2} \leq C$$

and similarly other estimates follow. To estimate  $\|\partial_t V^{\tau}\|_{L^2(0,T;L^2(\Omega))}^2$  we note that, whenever  $t \in (t_{n-1}, t_n]$ ,

$$\partial_t V^\tau = \frac{v^n_\delta - v^{n-1}_\delta}{\tau}$$

implying

$$\int_{0}^{T} \|\partial_{t}V^{\tau}\|^{2} dt = \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} \|\frac{v_{\delta}^{n} - v_{\delta}^{n-1}}{\tau}\|_{L^{2}(\Omega)}^{2} dt \leq \sum_{n=1}^{N} \tau \|\frac{v_{\delta}^{n} - v_{\delta}^{n-1}}{\tau}\|_{L^{2}(\Omega)}^{2} \leq C\tau N \leq C,$$

where we have used the estimate (5.5).

The proof for  $\partial_t U^{\tau}$  is the same as above and uses the estimate (5.8). The only remaining part in (5.31) is to show that  $\nabla \cdot \mathbf{Q}^{\tau} \in L^2(0,T; L^2(\Omega))$ . To see this note that

$$\nabla \cdot \mathbf{Q}^{\tau} = \nabla \cdot \mathbf{Q}_{\delta}^{n-1} + \frac{t - t_{n-1}}{\tau} \nabla \cdot (\mathbf{Q}_{\delta}^{n} - \mathbf{Q}_{\delta}^{n-1}).$$

Squaring both sides and using the elementary inequality

$$\|\nabla \cdot \mathbf{Q}^{\tau}\|_{L^{2}(\Omega)}^{2} \leq 2\|\nabla \cdot \mathbf{Q}_{\delta}^{n-1}\|^{2} + 2\frac{(t-t_{n-1})^{2}}{\tau^{2}}\|\nabla \cdot (\mathbf{Q}_{\delta}^{n} - \mathbf{Q}_{\delta}^{n-1})\|^{2}$$

integrating over t from 0 to T, since  $\nabla \cdot \mathbf{Q}_{\delta}^{n-1}$  and  $\nabla \cdot \mathbf{Q}_{\delta}^{n}$  are constant in  $(t_{n-1}, t_n)$  gives

$$\begin{split} \int_{0}^{T} \|\nabla \cdot \mathbf{Q}^{\tau}\|^{2} dt &\leq 2\tau \sum_{n=1}^{N} \|\nabla \cdot \mathbf{Q}_{\delta}^{n-1}\|^{2} + 2\sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} \frac{(t-t_{n-1})^{2}}{\tau^{2}} \|\nabla \cdot (\mathbf{Q}_{\delta}^{n} - \mathbf{Q}_{\delta}^{n-1})\|^{2} dt \\ &\leq 2\tau \sum_{n=1}^{N} \|\nabla \cdot \mathbf{Q}_{\delta}^{n-1}\|^{2} + 2\sum_{n=1}^{N} \frac{2\tau}{3} \|\nabla \cdot (\mathbf{Q}_{\delta}^{n} - \mathbf{Q}_{\delta}^{n-1})\|^{2}. \end{split}$$

Now use (5.10)–(5.11) to obtain

$$\int_{0}^{T} \|\nabla \cdot \mathbf{Q}^{\tau}\|^{2} dt \le C.$$

Note that the estimates above are uniform in  $\tau$ , if  $\delta = O(\sqrt{\tau})$  and we have  $(U^{\tau}, \mathbf{Q}^{\tau}, V^{\tau}, W^{\tau}) \in \mathcal{V} \times \mathcal{S} \times \mathcal{V} \times L^{\infty}(\Omega^{T})$ . Moreover, we have

LEMMA 5.7. A quadruple  $(u, \boldsymbol{Q}, v, w) \in \mathcal{V} \times \mathcal{S} \times \mathcal{V} \times L^{\infty}(\Omega^T)$  exists s.t. along a sequence  $\tau \searrow 0$  (and with  $\delta = O(\tau^{\frac{1}{2}})$ ) we have

- 1.  $U^{\tau} \rightharpoonup u$  weakly in  $L^{2}((0,T); L^{2}(\Omega)),$
- 2.  $\partial_t U^{\tau} \rightharpoonup \partial_t u$  weakly in  $L^2((0,T); L^2(\Omega)),$

Kumar, Pop, and Radu

3.  $\mathbf{Q}^{\tau} \rightarrow \mathbf{Q}$  weakly in  $L^{2}((0,T); L^{2}(\Omega)^{d}),$ 4.  $\nabla \cdot \mathbf{Q}^{\tau} \rightarrow \nabla \cdot \mathbf{Q}$  weakly in  $L^{2}((0,T); L^{2}(\Omega)),$ 5.  $V^{\tau} \rightarrow v$  weakly in  $L^{2}((0,T); L^{2}(\Omega)),$ 

- 6.  $\partial_t V^{\tau} \rightharpoonup \partial_t v$  weakly in  $L^2((0,T); L^2(\Omega))$ ,
- 7.  $W^{\tau} \rightharpoonup w$  weakly-star in  $L^{\infty}(\Omega)$ .

In the above only weak convergence of  $U^{\tau}$  in  $L^2(0,T;L^2(\Omega))$  is obtained, which is not sufficient for passing to the limit for non-linear term  $r(U^{\tau})$ . To obtain strong convergence, we use translation estimates as derived in Lemma 5.3.

LEMMA 5.8. It holds that

$$U^{\tau} \to u \text{ strongly in } L^2((0,T);L^2(\Omega)).$$

*Proof.* In view of  $\partial_t U^{\tau} \in L^2(0,T; L^2(\Omega))$ , the translation in time is already controlled. What we need is to control the translation in space. Due to [8] (Prop. 9.3, p.267), we need to prove that

$$\mathcal{I}_{\xi} := \int_{0}^{T} \int_{\Omega_{\xi}} \left| \triangle_{\xi} U^{\tau} \right|^{2} dx dt \to 0 \text{ as } |\xi| \searrow 0.$$

The definition of  $U^{\tau}$  immediately implies that

$$|\mathcal{I}_{\xi}| \leq \sum_{n=1}^{N} \tau \left( 2 \| \triangle_{\xi} u_{\delta}^{n} \|^{2} + 2 \| \triangle_{\xi} u_{\delta}^{n-1} \|^{2} \right).$$

Using Lemma 5.3 we find that

$$|\mathcal{I}_{\xi}| \le C|\xi|$$

where C is independent of  $\tau$  and  $\delta$ , implying the strong convergence.  $\Box$ 

To identify w with H(v) we further need the strong convergence of  $V^{\tau}$ . This is a consequence of lemmas 5.4 and 5.8.

LEMMA 5.9. For  $V^{\tau}$ , it holds that

$$V^{\tau} \to v \text{ strongly in } L^2((0,T);L^2(\Omega)).$$

*Proof.* Once again, we use the translation estimate and note that the regularity of  $\partial_t V^{\tau}$  ensures the control of the translation in time. What remains is to prove the following estimate

$$\mathcal{I}_{\xi} := \int_{0}^{T} \int_{\Omega_{\xi}} \left| \triangle_{\xi} V^{\tau} \right|^{2} dx dt \to 0 \text{ as } |\xi| \searrow 0.$$

Using the definition of  $V^{\tau}$  we have

$$\mathcal{I}_{\xi} \leq \sum_{n=1}^{N} \tau \left( 2 \| \triangle_{\xi} v_{\delta}^{n} \|^{2} + 2 \| \triangle_{\xi} v_{\delta}^{n-1} \|^{2} \right).$$

Thanks to Lemma 5.4 we have

$$\mathcal{I}_{\xi} \le C|\xi|$$

where C is independent of  $\tau$  and  $\delta$ , thus establishing the strong convergence.  $\Box$ 

14

Numerical Analysis

**5.4.** The limit equations. Once the strong convergence is obtained, the following theorem provides the existence of the weak solution in the mixed variational formulation.

THEOREM 5.10. The limit quadruple (u, Q, v, w) is a solution in the sense of Definition 4.1.

*Proof.* By the weak convergence, the estimates in Lemma 5.6 carry over for the limit quadruple  $(u, \mathbf{Q}, v, w)$ . Moreover, the time continuous approximation in (5.29) satisfies

$$\left(\partial_t U^{\tau}, \phi\right) + \left(\nabla \cdot \mathbf{Q}^{\tau}, \phi\right) + \left(\partial_t V^{\tau}, \phi\right) = \left(\nabla \cdot \left(\mathbf{Q}^{\tau} - \mathbf{Q}^n_{\delta}\right), \phi\right), \tag{5.32}$$

$$\left(\partial_t V^{\tau}, \theta\right) - \left(r(U^{\tau}) - W^{\tau}, \theta\right) = \left(H_{\delta}(V^{\tau}) - H_{\delta}(v_{\delta}^{n-1}, \theta) + \left(r(u_{\delta}^n) - r(U^{\tau}), \theta\right)$$
(5.33)

$$\mathbf{Q}^{\tau}, \boldsymbol{\psi}) - (U^{\tau}, \nabla \cdot \boldsymbol{\psi}) - (\mathbf{q}U^{\tau}, \boldsymbol{\psi}) = (\mathbf{Q}^{\tau} - \mathbf{Q}^{n}_{\delta}, \boldsymbol{\psi}) - (U^{\tau} - u^{n}_{\delta}, \nabla \cdot \boldsymbol{\psi}) - (\mathbf{q}(U^{\tau} - u^{n}_{\delta}), \boldsymbol{\psi})$$
(5.34)

for all  $(\phi, \theta, \psi) \in L^2(0, T; H^1_0(\Omega)), \mathcal{V}, \mathcal{S})$ . Note that, in fact, (5.32) also holds for  $\phi \in \mathcal{V}$ . Here we choose a better space to identify the limit, where we prove that the term on the right is vanishing along a sequence  $\tau \searrow 0$ . By density arguments, the limit will hold for  $\phi \in \mathcal{V}$ .

Consider first (5.32) and note that by Lemma 5.7, the left hand side converges to the desired limit. It only remains to show that the right hand side, denoted by  $\mathcal{I}_1$ , vanishes as  $\tau \searrow 0$ . Integrating by parts, which is allowed due to the choice of  $\phi \in L^2(0,T; H^1_0(\Omega))$ , one has

$$|\mathcal{I}_1| \le \left(\sum_{n=1}^N \tau C \|\mathbf{Q}_{\delta}^n - \mathbf{Q}_{\delta}^{n-1}\|^2\right)^{\frac{1}{2}} \left(\int_0^T \|\nabla \phi\|^2 dt\right)^{\frac{1}{2}}.$$

Due to the estimate (5.9),  $\sum_{n=1}^{N} \tau \|\mathbf{Q}_{\delta}^{n} - \mathbf{Q}_{\delta}^{n-1}\|^{2} \to 0.$ 

Next, we consider (5.33). First we prove that the last two integrals on the right hand side vanish, denoted by  $\mathcal{I}_2$  and  $\mathcal{I}_3$  vanish. For  $\mathcal{I}_2$  we use the Lipschitz continuity of  $H_{\delta}$  and the definition of  $V^{\tau}$  to obtain

$$|\mathcal{I}_{2}| \leq \left(\sum_{n=1}^{N} \frac{\tau}{\delta^{2}} \|v_{\delta}^{n} - v_{\delta}^{n-1}\|^{2}\right)^{\frac{1}{2}} \left(\int_{0}^{T} \|\theta\|^{2} dt\right)^{\frac{1}{2}}.$$

Using (5.5) we have

(

$$|\mathcal{I}_2| \le C \frac{\tau}{\delta} \left( \int_0^T \|\theta\|^2 dt \right)^{\frac{1}{2}}.$$

By the choice of  $\delta$ ,  $\frac{\tau}{\delta} \searrow 0$  as  $\tau \searrow 0$ , implying that  $\mathcal{I}_2$  vanishes in the limit.

For  $\mathcal{I}_3$  we use the Lipschitz continuity of r and (5.8) to get

$$|\mathcal{I}_3| \le \left(\sum_{n=1}^N \tau L_r \|u_{\delta}^n - u_{\delta}^{n-1}\|^2\right)^{\frac{1}{2}} \left(\int_0^T \|\psi\|^2 dt\right)^{\frac{1}{2}} \to 0.$$

For the first term on the left in (5.32), the limit is straightforward. For the limit of the second term, with strong convergence of  $U^{\tau}$  and weak-\* convergence of  $W^{\tau}$  we get

$$\lim_{\tau \searrow 0} \left( r(U^{\tau}) - W^{\tau}, \theta \right) = \left( r(u) - w, \theta \right),$$

leading to the limiting equation

$$(\partial_t v, \theta) = (r(u) - w, \theta) \text{ for all } \theta \in \mathcal{V}.$$
(5.35)

Now we consider (5.34) and denote the corresponding integrals on the right hand side respectively by  $\mathcal{I}_4, \mathcal{I}_5$ , and  $\mathcal{I}_6$ . By the definition of  $\mathbf{Q}^{\tau}$  and (5.9), as  $\tau \searrow 0$  we obtain

$$|\mathcal{I}_4| \le \left(\sum_{n=1}^N \tau \|\mathbf{Q}_{\delta}^n - \mathbf{Q}_{\delta}^{n-1}\|^2\right)^{\frac{1}{2}} \left(\int_0^T \|\boldsymbol{\psi}\|^2 dt\right)^{\frac{1}{2}} \to 0.$$

Similarly, for  $\mathcal{I}_5$  and  $\mathcal{I}_6$ , using (5.8)

$$|\mathcal{I}_{5}| \leq \left(\sum_{n=1}^{N} \tau \|u_{\delta}^{n} - u_{\delta}^{n-1}\|^{2}\right)^{\frac{1}{2}} \left(\int_{0}^{T} \|\psi\|^{2} dt\right)^{\frac{1}{2}} \to 0, \text{ and}$$

$$|\mathcal{I}_{6}| \leq \left(\sum_{n=1}^{N} \tau M_{q}^{2} \| u_{\delta}^{n} - u_{\delta}^{n-1} \|^{2}\right)^{\frac{1}{2}} \left(\int_{0}^{T} \| \boldsymbol{\psi} \|^{2} dt\right)^{\frac{1}{2}} \to 0$$

With this the limit equation takes the form

$$(\mathbf{Q}, \boldsymbol{\psi}) - (u, \nabla \cdot \boldsymbol{\psi}) - (\mathbf{q}u, \boldsymbol{\psi}) = 0.$$
(5.36)

To conclude the proof what remains is to show that w = H(v). Since we have  $V^{\tau}$  strongly converging, we also obtain  $V^{\tau} \to v$  pointwise a.e. and further, as  $\tau \searrow 0$ , by construction  $\delta \searrow 0$ . For the set  $R_+ := \{(t, x) : v(t, x) > 0\}$ , let us assume  $\mu := v(t, x, z)/2 > 0$ . Then the pointwise convergence implies the existence of a  $\varepsilon_{\mu} > 0$  such that  $V^{\tau} > \mu$  for all  $\varepsilon \leq \varepsilon_{\mu}$ . Then for any  $\varepsilon \leq \varepsilon_{\mu}$  we have  $W^{\tau} = 1$  implying w = 1. A similar conclusion also holds for  $R_-$  where  $R_- := \{(t, x) : v(t, x) < 0\}$ .

For the case when v = 0; consider the set  $R_0 := \{(t, x, z) : v(t, x, z) = 0\}$ . Now in the interior of the set  $R_0$ ,  $\partial_t v = 0$ . Next, from the weak convergence of  $\partial_t V^{\tau}$ ,  $W^{\tau}$ ,  $r(U^{\tau})$ , we have the following limit equation

$$(\partial_t v, \theta) = (r(u) - w, \theta).$$

Hence, for the interior of the set  $R_0$ , we obtain w = r(u). Furthermore, the bounds  $0 \le W^{\tau} \le 1$  with weak- convergence of  $W_h^{\tau}$  to w imply the same bounds on w and hence w = r(u) with  $0 \le r(u) \le 1$ .  $\Box$ 

6. The mixed finite element formulation. Following the semi-discrete scheme, we now consider the fully discrete system (discretized in both space and time) and show the convergence of the numerical method. In particular, we consider the mixed finite element discretization in space and for the time we retain the discretization as in the semi-discrete case. The steps for the proof of convergence are similar to the semi-discrete situation and where ever the proof is similar to time-discrete case treated above, we suppress the details. Further, to simplify notation, henceforth, we suppress the subscript  $\delta$ .

The fully discrete formulation for the weak solution of (2.1)–(2.2) builds on the time discretization in (5.2), and consider a uniform time stepping that is implicit in u and explicit in v. For the space discretization, we have  $\Omega$  decomposed in 2– dimensional simplices (triangles) denoted by  $\mathcal{T}_h$  and having the mesh-size h. We assume  $\Omega$  to be polygonal as has been stated in Section 3. The function spaces used here are already introduced in Section 3.

Starting with  $u_h^0 = u_I, v_h^0 = v_I$ , with  $n \in \{1, \ldots, N\}$ , the approximation  $(u_h^n, v_h^n, \mathbf{Q}_h^n, w_h^n)$  of  $(u(t_n), v(t_n), \mathbf{Q}(t_n), w(t_n))$  at  $t = t_n$  solves :

Problem 
$$\mathbf{P}_h^n$$
: Given  $(u_h^{n-1}, v_h^{n-1}) \in (\mathcal{V}_h, \mathcal{V}_h)$  find  $(u_h^n, v_h^n, \mathbf{Q}_h^n, w_h^n) \in (\mathcal{V}_h, \mathcal{V}_h, \mathcal{S}_h, L^{\infty}(\Omega))$  satisfying

$$\begin{aligned} (u_{h}^{n} - u_{h}^{n-1}, \phi) &+ \tau (\nabla \cdot \mathbf{Q}_{h}^{n}, \phi) + (v_{h}^{n} - v_{h}^{n-1}, \phi) = 0, \\ (v_{h}^{n} - v_{h}^{n}, \theta) &- \tau (r(u_{h}^{n}), \theta) - \tau (H_{\delta}(v_{h}^{n-1}), \theta) = 0, \\ (\mathbf{Q}_{h}^{n}, \psi) - (u_{h}^{n}, \nabla \cdot \psi) - (\mathbf{q}_{h}u_{h}^{n}, \psi) = 0, \end{aligned}$$
(6.1)

for all  $(\phi, \theta, \psi) \in \mathcal{V}_h \times \mathcal{V}_h \times \mathcal{S}_h$ . For completion, we define

$$w_h^n = H_\delta(v_h^n).$$

For stability reasons, as before, we choose  $\delta = O(\tau^{\frac{1}{2}})$  (see [14, 26] for detailed arguments).

The fully discrete scheme (6.1) seeks solution on a finite dimensional vector space for any given discretization parameters. From (6.1)<sub>1</sub> and (6.1)<sub>2</sub>, we eliminate  $v_h^n$ , which is computed after having obtained  $(u_h^n, \mathbf{Q}_h^n)$  satisfying for all  $(\phi, \psi) \in (\mathcal{V}_h, \mathcal{S}_h)$ 

$$\begin{aligned} (u_{h}^{n} - u_{h}^{n-1}, \phi) + \tau (\nabla \cdot \mathbf{Q}_{h}^{n}, \phi) + \tau (r(u_{h}^{n}) - H_{\delta}(v_{h}^{n-1}), \phi) &= 0, \\ (\mathbf{Q}_{h}^{n}, \psi) - (u_{h}^{n}, \nabla \cdot \psi) - (\mathbf{q}_{h}u_{h}^{n}, \psi) &= 0. \end{aligned}$$
(6.2)

In the above formulation, the nonlinearities only involve  $u_h^n$ ; the  $H_\delta$  is known, from the previous time step and is in  $L^{\infty}$ .

The existence follows from [37], Theorem 4.3, which treats a more general case. Its proof is based on [42] (Lemma 1.4, p.140). Following the ideas in Section 5, one can prove that (6.2) has a unique solution pair  $(u_h^n, \mathbf{Q}_h^n)$ . This also determines  $v_h^n$  and  $w_h^n$  uniquely. We summarize the above result

LEMMA 6.1. Problem  $\boldsymbol{P}_h^n$  has a unique solution pair  $(u_h^n, \boldsymbol{Q}_h^n, v_h^n, w_h^n)$ .

**6.1. The a priori estimates.** We proceed with the energy estimates which are analogous to the semi-discrete case. We simply state the results as their proof follows as in the semi-discrete case.

LEMMA 6.2. The following estimates hold

$$\sup_{k=1,\dots,N} \left\| u_h^k \right\| \le C \tag{6.3}$$

$$\left\| v_h^n - v_h^{n-1} \right\| \le C\tau \tag{6.4}$$

$$\sup_{k=1,\dots,N} \left\| v_h^k \right\| \le C \tag{6.5}$$

$$\sup_{k=1,\dots,N} \left\| \boldsymbol{Q}_h^k \right\| \le C \tag{6.6}$$

$$\sum_{n=1}^{N} \left\| u_{h}^{n} - u_{h}^{n-1} \right\|^{2} \le C\tau \tag{6.7}$$

$$\sum_{n=1}^{N} \left\| \boldsymbol{Q}_{h}^{n} - \boldsymbol{Q}_{h}^{n-1} \right\|^{2} \le C$$
(6.8)

$$\sum_{n=1}^{N} \tau \left\| \nabla \cdot \boldsymbol{Q}_{h}^{n} \right\|^{2} \le C \tag{6.9}$$

$$\sum_{n=1}^{N} \tau \left\| \nabla \cdot (\boldsymbol{Q}_{h}^{n} - \boldsymbol{Q}_{h}^{n-1}) \right\|^{2} \leq C$$
(6.10)

We continue with the steps analogous to the semi-discrete situation. As in (5.29) we consider the time-continuous approximation by the piecewise linear interpolations of the time discrete solutions. With  $t \in [t_{n-1}, t_n]$ , define

$$Z_h^{\tau}(t) := \frac{(t - t_{n-1})}{\tau} z_h^n + \frac{(t_n - t)}{\tau} z_h^{n-1}, \tag{6.11}$$

(6.12)

where  $z_h^n, z_h^{n-1}$  are the time-discrete solutions from which we construct the corresponding timecontinuous approximation  $Z_h^{\tau}$ . The symbol z may be replaced here by either u, v, or **Q**, and the same holds for Z. As before, the estimates in Lemma 6.2 carry over for the time-continuous approximation (the proof is omitted) and we obtain

LEMMA 6.3. The time-continuous approximations satisfy the following estimates

$$\|\partial_t U_h^{\tau}\|^2 + \|\nabla \cdot \mathbf{Q}_h^{\tau}\|^2 + \|U_h^{\tau}\|^2 + \|V_h^{\tau}\|^2 + \|\mathbf{Q}_h^{\tau}\|^2 \le C,$$
(6.13)

0

$$\leq W_h^\tau \leq 1. \tag{6.14}$$

Here the norms are taken with respect to  $L^2(0,T;L^2(\Omega))$ . The estimates are uniform in  $\tau$  and  $\delta$  and furthermore we have  $(U_h^{\tau}, \mathbf{Q}_h^{\tau}, V_h^{\tau}, W_h^{\tau}) \in \mathcal{V} \times \mathcal{S} \times \mathcal{V} \times L^{\infty}(\Omega)$ . Clearly, if  $\tau \searrow 0$  with  $\delta = O(\tau^{\frac{1}{2}})$  implies that both  $\delta, \frac{\tau}{\delta} \searrow 0$ . The compactness arguments from the Lemma 6.3 lead to the following convergence result:

- LEMMA 6.4. Along a sequence  $\tau \searrow 0$ , it holds that
- 1.  $U_h^{\tau} \rightharpoonup u$  weakly in  $L^2((0,T); L^2(\Omega))$ ,
- 2.  $\partial_t U_h^{\tau} \rightharpoonup \partial_t u$  weakly in  $L^2((0,T); H^{-1}(\Omega))$ ,
- 3.  $\boldsymbol{Q}_{h}^{\tau} \rightharpoonup \boldsymbol{Q}$  weakly in  $L^{2}((0,T); L^{2}(\Omega)^{d}),$

- 4.  $\nabla \cdot \boldsymbol{Q}_{h}^{\tau} \rightharpoonup \chi$  weakly in  $L^{2}((0,T); L^{2}(\Omega)),$ 5.  $V_{h}^{\tau} \rightharpoonup v$  weakly in  $L^{2}((0,T); L^{2}(\Omega)),$ 6.  $\partial_{t}V_{h}^{\tau} \rightharpoonup \partial_{t}v$  weakly in  $L^{2}((0,T); L^{2}(\Omega)),$
- 7.  $W_h^{\tau} \rightharpoonup w$  weakly-star in  $L^{\infty}(\Omega)$ .

As in the semi-discrete case, identification of the above limit  $\chi$  with  $\nabla \cdot \mathbf{Q}$  is obtained via smooth test functions. Note that the above lemma only provides weak convergence for  $U_h^{\tau}, V_h^{\tau}$ ; in the wake of nonlinearities, the strong convergence is needed. However, the techniques from the semi-discrete case can not be applied directly. This is because the translation of a function that is piecewise constant on the given mesh need not be piecewise constant on that mesh. We therefore adopt the finite volume framework in [19] in order to overcome this difficulty.

6.2. Strong convergence. In what follows, we establish the required strong convergence of  $U_h^{\tau}$  followed by that of  $V_h^{\tau}$ . We provide the notations used below in the framework of finite volumes. Let  $\mathcal{E}$  denote the set of edges of the simplices  $\mathcal{T}_h$ . Also, we have that  $\mathcal{E} = \mathcal{E}_{int} \cup \mathcal{E}_{ext}$ with  $\mathcal{E}_{ext} = \mathcal{E} \bigcap \partial \Omega$  and  $\mathcal{E}_{int} = \mathcal{E} \setminus \mathcal{E}_{ext}$ . We adopt the following notation:

$$\begin{aligned} |T| &- \text{ the area of } T \in \mathcal{T}_h, \\ \mathbf{x}_i &- \text{ the centre of the circumcircle of } T, \\ l_{ij} &- \text{ the edge between } T_i \text{ and } T_j, \\ d_{ij} &- \text{ the distance from } \mathbf{x}_i \text{ to } l_{ij}, \\ \sigma_{ij} &- \frac{|l_{ij}|}{d_{ij}}, \end{aligned}$$
(6.15)

In analogy with the spatially continuous case, we define the following discrete inner product for any  $u_h^n, v_h^n \in \mathcal{V}_h$ 

$$(u_h^n, v_h^n)_h := \sum_{T_i \in \mathcal{T}_h} |T_i| u_{h,i}^n v_{h,i}^n, \quad (u_h^n, v_h^n)_{1,h} := \sum_{l_{ij} \in \mathcal{E}} |\sigma_{ij}| (u_{h,i}^n - u_{h,j}^n) (v_{h,i}^n - v_{h,j}^n).$$
(6.16)

The discrete inner product gives rise to discrete  $H_0^1$  norm, which is

$$\|u_h^n\|_{1,h} = \sum_{l_{ij} \in \mathcal{E}} |\sigma_{ij}| (u_{h,i}^n - u_{h,j}^n)^2.$$
(6.17)

In [19], the following discrete Poincare inequality is proved

$$\|u_h^n\| \le C \|u_h^n\|_{1,h},\tag{6.18}$$

with C independent of h or  $u_h^n$ . Based on Lemma 4 in [19], below we show that the translations are controlled by the discrete  $\|\cdot\|_{1,h}$  norm.

LEMMA 6.5. Let  $\Omega$  be an open bounded set of  $\mathbb{R}^2$  and let  $\mathcal{T}_h$  be an admissible mesh. For a given u defined in  $\Omega$  and extended to  $\overline{u}$  by 0 outside  $\Omega$  we have

$$\|\triangle_{\xi}\bar{u}\|_{L^{2}(\mathbb{R}^{2})}^{2} \leq \|u\|_{1,h}^{2}|\xi|(|\xi|+C\operatorname{size}(\mathcal{T}_{h})), \text{ for all } \xi \in \mathbb{R}^{2}.$$
(6.19)

This shows that for a sequence  $\{u_h^n\}$  having the discrete  $H_0^1$  norm uniformly bounded, the  $L^2$ norm of the translations  $\triangle_{\xi} u_h^n$  vanishes uniformly with respect to h as  $\eta \searrow 0$ . This is an essential step in proving the strong  $L^2$ - convergence for  $u_h^n$ . Here we only need to show that  $u_h^n$  has bounded discrete  $H_0^1$  norm

LEMMA 6.6. For the sequence  $u_h^n$ , the following inequality holds uniformly with respect to h,

$$\|u_h^n\|_{1,h} \le C(\|\boldsymbol{Q}_h^n\| + \|u_h^n\|).$$
(6.20)

*Proof.* The approach is inspired from the semi-discrete situation and is adapted to the present context by defining appropriate test function. Define

$$|T_i|f_h^n(T_i) := \sum_{l_{ij}} \frac{|l_{ij}|}{d_{ij}} (u_{h,i}^n - u_{h,j}^n)$$
(6.21)

and note that by the definition of  $\|\cdot\|_{1,h}^2$ ,

$$(f_h^n, u_h^n) = \sum_i T_i f_h^n(T_i) u_h^n(T_i) = \sum_{l_{ij}} \frac{|l_{ij}|}{d_{ij}} |u_{h,i}^n - u_{h,j}^n|^2 = ||u_h^n||_{1,h}^2.$$
(6.22)

Further, by using Cauchy-Schwarz we obtain

$$\|f_h^n\|_{L^2(\Omega)}^2 = \sum_i |T_i| |f_h^n(T_i)|^2 \le \sum_{l_{ij}} \frac{|l_{ij}|}{d_{ij}} (u_i^n - u_j^n)^2 \frac{1}{|T_i|} \sum_{l_{ij}} \frac{|l_{ij}|}{d_{ij}}$$

which implies that

$$\|f_h^n\| \le \|u_h^n\|_{1,h}.$$
(6.23)

Note that  $f_h^n \in L^2(\Omega)$  and hence, there exists  $\psi_h \in \mathcal{S}_h$  which satisfies

$$\nabla \cdot \boldsymbol{\psi}_h = f_h^n \quad \text{in} \quad \Omega, \tag{6.24}$$

$$\boldsymbol{\psi}_h = 0 \quad \text{on} \quad \boldsymbol{\Gamma}. \tag{6.25}$$

By (6.23), it also holds that

$$\|\psi_h\|_{L^2(\Omega)} \le C \|f_h^n\|_{L^2(\Omega)} \le C \|u_h^n\|_{1,h}.$$
(6.26)

Now choose for the test function  $\psi = \psi_h$  in (6.1)<sub>3</sub>

$$(\mathbf{Q}_h^n, \boldsymbol{\psi}_h) - (u_h^n, \nabla \cdot \boldsymbol{\psi}_h) - (\mathbf{q}_h u_h^n, \boldsymbol{\psi}_h) = 0.$$

Note that by (6.22)

$$(u_h^n, \nabla \cdot \psi_h) = (u_h^n, f_h^n) = \|u_h^n\|_{1,h}^2$$

This implies that

$$\begin{aligned} \|u_{h}^{n}\|_{1,h}^{2} &= (u_{h}^{n}, \nabla \cdot \psi_{h}) = (\mathbf{Q}_{h}^{n}, \psi_{h}) - (\mathbf{q}_{h}u_{h}^{n}, \psi_{h}) \\ &\leq \|\mathbf{Q}_{h}^{n}\|\|\psi_{h}\| + M_{q}\|u_{h}^{n}\|\|\psi_{h}\| \leq C\|\mathbf{Q}_{h}^{n}\|\|u_{h}^{n}\|_{1,h} + CM_{q}\|u_{h}^{n}\|\|u_{h}^{n}\|_{1,h} \end{aligned}$$

and the conclusion follows.  $\Box$ 

#### Kumar, Pop, and Radu

In view of the above lemma, obtaining the relative compactness in  $L^2$  is straightforward.

LEMMA 6.7. Along a sequence  $(\tau, h)$  converging to (0, 0) (and with  $\delta = O(\sqrt{\tau})$ ),  $U_h^{\tau}$  converges strongly in  $L^2(0, T; L^2(\Omega))$ .

*Proof.* Since  $\partial_t U_h^{\tau}$  is in  $L^2$ , the translation with respect to time is already controlled. What remains is to consider the translation with respect to space. Take (6.20) and sum over  $n = 1, \ldots, N$  to obtain

$$\tau \sum_{n=1}^{N} \|u_h^n\|_{1,h}^2 \le C\tau \sum_{n=1}^{N} (\|Q_h^n\|^2 + \|u_h^n\|^2) \le C$$
(6.27)

and using (6.3) and (6.6) gives

$$\tau \sum_{n=1}^{N} \|u_h^n\|_{1,h}^2 \le C$$

Now use Lemma 6.5 to control the translations by the  $\|\cdot\|_{1,h}$  norm (after extending  $u_h^n$  by 0 outside  $\Omega$ ; for simplicity retain the same notation)

$$\tau \sum_{n=1}^{N} \|u_{h}^{n}(\cdot + \xi) - u_{h}^{n}\|_{L^{2}(\mathbb{R}^{2})}^{2} \leq C|\xi|(|\xi| + \operatorname{size}(\mathcal{T}_{h})),$$

which, in turn, provides similar estimate for  $U_h^{\tau}$ 

$$\tau \sum_{n=1}^{N} \|U_{h}^{\tau}(\cdot + \xi) - U_{h}^{\tau}\|_{L^{2}(\mathbb{R}^{2})}^{2} \leq C|\xi|(|\xi| + \operatorname{size}(\mathcal{T}_{h})).$$

The Kolomogorov compactness theorem proves the assertion.  $\Box$ 

The strong convergence of  $U_h^{\tau}$  gives the strong convergence of  $V_h^{\tau}$ .

LEMMA 6.8. Along a sequence  $(\tau, h)$  converging to (0, 0),  $V_h^{\tau}$  converges strongly to v in  $L^2(0, T; L^2(\Omega))$ .

*Proof.* As before, the translations with respect to time are already controlled by virtue of  $\partial_t V_h^{\tau} \in L^2$ . We now consider the case for the translation with respect to space. Since both  $u_h^n, v_h^n$  are piecewise constants in each simplex T, we have for every  $x \in T$ 

$$v_h^n(x) = v_h^{n-1}(x) + \tau \left( r(u_h^n(x)) - \tau H_\delta(v_h^{n-1}(x)) \right)$$
$$v_h^n(x+\xi) = v_h^{n-1}(x+\xi) + \tau \left( r(u_h^n(x+\xi)) - \tau H_\delta(v_h^{n-1}(x+\xi)) \right)$$

so that for any  $x \in \Omega_{\xi}$  we have

$$\triangle_{\xi}(v_h^n - v_h^{n-1}) = \tau \triangle_{\xi} r(u_h^n) - \tau \triangle_{\xi} H_{\delta}(v_h^{n-1}).$$

Multiplying by  $riangle_{\xi} v_h^n$  and rewriting the left hand side, we have

$$\frac{1}{2} \left\{ \left| \bigtriangleup_{\xi} v_h^n \right|^2 - \left| \bigtriangleup_{\xi} v_h^{n-1} \right|^2 + \left| \bigtriangleup_{\xi} (v_h^n - v_h^{n-1}) \right|^2 \right\}$$

$$\leq \tau L_r \left| \bigtriangleup_{\xi} u_h^n \right| \left| \bigtriangleup_{\xi} v_h^n \right| - \tau \left( \bigtriangleup_{\xi} H_{\delta}(v_h^{n-1}) \right) \bigtriangleup_{\xi} v_h^n.$$
(6.28)

The term involving the  $\triangle_{\xi} H_{\delta}$  can be rewritten as

$$\left(\triangle_{\xi}H_{\delta}(v_{h}^{n-1})\right)\triangle_{\xi}v_{h}^{n}=\left(\triangle_{\xi}H_{\delta}(v_{h}^{n-1})\right)\triangle_{\xi}v_{h}^{n-1}+\left(\triangle_{\xi}H_{\delta}(v_{h}^{n-1})\right)\left(\triangle_{\xi}(v_{h}^{n}-v_{h}^{n-1})\right)$$

and due to monotonicity of  $H_{\delta}$ , we have

$$\left(\triangle_{\xi} H_{\delta}(v_h^{n-1})\right) \triangle_{\xi} v_h^{n-1} \ge 0.$$

20

Numerical Analysis

Using above in (6.28) gives

$$\frac{1}{2} \left\{ |\triangle_{\xi} v_{h}^{n}|^{2} - |\triangle_{\xi} v_{h}^{n-1}|^{2} + |\triangle_{\xi} (v_{h}^{n} - v_{h}^{n-1})|^{2} \right\} \\ \leq \tau L_{r}^{2} |\triangle_{\xi} u_{h}^{n}|^{2} + \frac{1}{4} |\triangle_{\xi} v_{h}^{n}|^{2} + \frac{1}{4} |\triangle_{\xi} (v_{h}^{n} - v_{h}^{n-1})|^{2} + \frac{\tau^{2}}{\delta^{2}} |\triangle_{\xi} v_{h}^{n-1}|^{2}.$$

Integrating over  $\Omega_{\xi}$  and summing over  $n = 1, \dots, k$  for any  $k \in \{1, \dots, N\}$  gives

$$\frac{1}{2} \| \triangle_{\xi} v_{h}^{k} \|^{2} + \frac{1}{4} \sum_{n=1}^{k} \| \triangle_{\xi} (v_{h}^{n} - v_{h}^{n-1}) \|^{2} \\
\leq \| \triangle_{\xi} v_{I,h} \|^{2} + \tau \sum_{n=1}^{k} L_{r}^{2} \| \triangle_{\xi} u_{h}^{n} \|^{2} + \frac{1}{4} \tau \sum_{n=1}^{k} \| \triangle_{\xi} v_{h}^{n} \|^{2} + \sum_{n=1}^{k} \frac{\tau^{2}}{\delta^{2}} \| \triangle_{\xi} v_{h}^{n-1} \|^{2},$$

where the norms are taken with respect to  $\Omega_{\xi}$ . Choosing  $\delta = O(\tau^{\frac{1}{2}})$  leads to

$$\frac{1}{2} \|\Delta_{\xi} v_h^k\|^2 + \frac{1}{4} \sum_{n=1}^k \|\Delta_{\xi} (v_h^n - v_h^{n-1})\|^2 \le \|\Delta_{\xi} v_{I,h}\|^2 + \tau \sum_{n=1}^k L_r^2 \|\Delta_{\xi} u_h^n\|^2 + C\tau \sum_{n=1}^k \|\Delta_{\xi} v_h^n\|^2.$$

Applying the Gronwall lemma provides

$$\sup_{k=1,\dots,N} \|\Delta_{\xi} v_h^k\|^2 \le C \|\Delta_{\xi} v_{I,h}\|^2 + \tau \sum_{n=1}^N \|\Delta_{\xi} u_h^n\|^2$$

The strong convergence of  $U_h^{\tau}$  in  $L^2(0,T; L^2(\Omega))$  implies that the last term vanishes in the limit of  $|\xi| \searrow 0$  (see the proof of Lemma 6.7).

To estimate the translations for the initial condition we consider  $v_{I,h}$  as the finite volume approximation of  $v_I$  defined (formally) by

$$-\Delta v_{I,h} = -\Delta v_I, \quad \text{in } \Omega$$

with homogenous Dirichlet boundary conditions. This implies

$$\|v\|_{1,h} \le C \|\nabla v_I\| \le C.$$

Since the translations are approaching 0 if  $||v_{I,h}||_{1,h} \leq C$  (uniformly in h),  $||\Delta_{\xi}v_{I,h}|| \to 0$  as  $|\xi| \searrow 0$ . From the above we conclude that  $||\Delta_{\xi}v_{h}^{k}||^{2} \to 0$  as  $|\xi|$  goes to 0.

Finally, note that the definition of  $V_h^\tau$  implies the rough estimate

$$\int_{0}^{T} \|\triangle_{\xi} V_{h}^{\tau}\|^{2} dt \leq 2\tau \sum_{n=1}^{N} \|\triangle_{\xi} v_{h}^{n}\|^{2} + 2\tau \sum_{n=1}^{N} \|\triangle_{\xi} v_{h}^{n-1}\|^{2},$$

and the right hand side vanishes uniformly in h as  $|\xi| \searrow 0$ , hence  $V_h^{\tau}$  converges strongly.  $\Box$ 

**6.3. The limit equations.** Up to now we obtained the convergence of the fully discrete triples  $(U_h^{\tau}, V_h^{\tau}, \mathbf{Q}_h^{\tau})$  along a sequence  $(\tau, h)$  approaching (0, 0) with  $\delta = O(\sqrt{\tau})$ . Clearly, the  $(L^{\infty} \text{ weakly}^*)$  convergence extends to the sequence  $W_h^{\tau} = H_{\delta}(V_h^{\tau})$ . In what follows, we identify the limit discussed in the preceding section as the weak formulation (4.1).

THEOREM 6.9. The limit quadruple  $(u, \mathbf{Q}, v, w)$  is a weak solution in the sense of Definition 4.1.

*Proof.* By the weak convergence, the estimates in Lemma 6.3 carry over for the limit triple  $(u, \mathbf{Q}, v)$ . By  $(6.1)_1$  we have

$$\int_{0}^{T} (\partial_{t} U_{h}^{\tau}, \phi) dt + \int_{0}^{T} (\nabla \cdot \mathbf{Q}_{h}^{\tau}, \phi) dt + \int_{0}^{T} (\partial_{t} V_{h}^{\tau}, \phi) dt$$

$$= \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (\partial_{t} U_{h}^{\tau}, \phi - \phi_{h}) dt + \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (\nabla \cdot \mathbf{Q}_{h}^{\tau} - \nabla \cdot \mathbf{Q}_{h}^{n}, \phi) dt$$

$$+ \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (\nabla \cdot \mathbf{Q}_{h}^{\tau}, \phi - \phi_{h}) dt + \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (\nabla \cdot \mathbf{Q}_{h}^{\tau} - \nabla \cdot \mathbf{Q}_{h}^{n}, \phi_{h} - \phi) dt$$

$$+ \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (\partial_{t} V_{h}^{\tau}, \phi - \phi_{h}) dt.$$
(6.29)

for all  $\phi \in L^2(0, T; H_0^1(\Omega))$ , and where  $\phi_h$  is the projection  $\phi_h = P\phi$  introduced in Section 3. Note that we assume again an  $H^1$  regularity in space for the test function  $\phi$ . We use this to control the terms involving  $\|\phi - \phi_h\|$  by using the property (3.1). A usual density argument lets the result hold for all  $\phi \in \mathcal{V}$ .

The left hand side gives the desired limit terms; it only remains to show that the right hand side vanishes in the limit. Denote the successive integrals on the right by  $\mathcal{I}_i$ ,  $i = 1, \ldots, 5$ . We deal with each term separately.

For  $\mathcal{I}_1$  we use (6.13) to obtain that as  $h \searrow 0$ 

$$|\mathcal{I}_1| \le \|\partial_t U_h^\tau\|_{L^2(0,T;L^2(\Omega))} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\phi - \phi_h\|_{L^2(\Omega)}^2 dt\right)^{\frac{1}{2}} \le Ch \|\nabla\phi\|_{L^2(0,T;L^2(\Omega))} \to 0.$$

Similarly, by (6.8), for  $\mathcal{I}_2$  one gets

$$|\mathcal{I}_2| \le \left(\sum_{n=1}^N \tau \|\mathbf{Q}_h^n - \mathbf{Q}_h^{n-1}\|^2\right)^{\frac{1}{2}} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\nabla \phi\|_{L^2(\Omega)}^2 dt\right)^{\frac{1}{2}} \le C\tau^{\frac{1}{2}}.$$

Clearly  $\mathcal{I}_2$  vanishes in the limit of  $\tau \searrow 0$ . Next, for  $\mathcal{I}_3$ , we have

$$|\mathcal{I}_3| \le \|\nabla \cdot \mathbf{Q}_h^{\tau}\|_{L^2(0,T;L^2(\Omega))} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\phi - \phi_h\|^2 dt\right)^{\frac{1}{2}} \le Ch \|\nabla \phi\|_{L^2(0,T;L^2(\Omega))}$$

using (6.13). Hence,  $\mathcal{I}_3$  goes to 0 as  $h \searrow 0$ . Proceeding in the similar way, for  $\mathcal{I}_4$ 

$$|\mathcal{I}_4| \le \left(\sum_{n=1}^N \tau \|\nabla \cdot \mathbf{Q}_h^n - \nabla \cdot \mathbf{Q}_h^{n-1}\|^2\right)^{\frac{1}{2}} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\phi - \phi_h\|_{L^2(\Omega)}^2 dt\right)^{\frac{1}{2}} \le Ch \|\nabla \phi\|_{L^2(0,T;L^2(\Omega))}$$

by using (6.10) implying that  $\mathcal{I}_4$  vanishes in the limit.

In the same manner, for  $\mathcal{I}_5$  we use the bounds for  $\partial_t V_h^{\tau}$  and obtain

$$|\mathcal{I}_5| \le \|\partial_t V_h^{\tau}\|_{L^2(0,T;L^2(\Omega))} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\phi - \phi_h\|_{L^2(\Omega)}^2 dt\right)^{\frac{1}{2}} \le Ch \|\nabla\phi\|_{L^2(0,T;L^2(\Omega))}.$$

Next we consider  $(6.1)_2$ , which we rewrite as

$$\begin{split} &\int_{0}^{T} (\partial_{t} V_{h}^{\tau}, \theta) dt - \int_{0}^{T} \left( r(U_{h}^{\tau}) - W_{h}^{\tau}, \theta \right) dt \\ &= \int_{0}^{T} \left( \partial_{t} V_{h}^{\tau}, \theta - \theta_{h} \right) dt + \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} \left( H_{\delta}(V_{h}^{\tau}) - H_{\delta}(v_{h}^{n-1}), \theta \right) dt \\ &+ \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} \left( H_{\delta}(v_{h}^{n-1}), \theta - \theta_{h} \right) dt + \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} \left( r(u_{h}^{n}) - r(U_{h}^{\tau}), \theta \right) dt \\ &+ \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} \left( r(u_{h}^{n}), \theta_{h} - \theta \right) dt. \end{split}$$

for  $\theta \in L^2(0, T; H_0^1(\Omega))$  and  $\theta_h$  is the  $P_h$  projection of  $\theta$ . A better regularity of  $\theta$  is again chosen for identifying the limits and controlling the errors due to the projections. We would retrieve the desired limiting equations once we prove that the integrals on the right hand side vanish. Let us denote the successive integrals by  $\mathcal{I}_i$ ,  $i = 1, \ldots, 5$  respectively. For  $\mathcal{I}_1$  we get by using (6.13) and recalling the projection estimate (3.1)

$$|\mathcal{I}_1| \le \left(\int_0^T \|\partial_t V_h^{\tau}\|^2 dt\right)^{\frac{1}{2}} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|(\theta - \theta_h)\|^2 dt\right)^{\frac{1}{2}} \le Ch \|\theta\|_{L^2(0,T;H^1_0(\Omega))}$$

which vanishes in the limit as  $h \searrow 0$ . For  $\mathcal{I}_2$ , we use the definition of  $W^{\tau}$  and Lipschitz continuity of  $H_{\delta}$  to obtain

$$|\mathcal{I}_2| \le \sum_{n=1}^N \tau \frac{1}{\delta} \|v_h^n - v_h^{n-1}\| \|\theta\| \le \sum_{n=1}^N \tau C \frac{\tau}{\delta} \|\theta\|$$

by using (6.4) and further using  $\tau/\delta \searrow 0$  by the construction of  $\delta$  we obtain  $\mathcal{I}_2 \to 0$ . Next, we consider  $\mathcal{I}_3$ 

$$|\mathcal{I}_{3}| \leq C \left( \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} \|\theta - \theta_{h}\|^{2} dt \right)^{\frac{1}{2}} \leq Ch \|\nabla \theta\|_{L^{2}(0,T;L^{2}(\Omega))} \to 0 \quad \text{as} \quad h \searrow 0$$

because of (3.1). To continue,

$$|\mathcal{I}_4| \le \left(\sum_{n=1}^N \tau L_r^2 \|u_h^n - u_h^{n-1}\|^2\right)^{\frac{1}{2}} \left(\sum_{n=1}^N \tau \|\theta_h\|^2\right)^{\frac{1}{2}}$$

and using the estimate (6.7), we obtain  $\mathcal{I}_4 \to 0$ . For  $\mathcal{I}_5$ , as  $h \searrow 0$ ,

$$|\mathcal{I}_5| \le L_r \left(\sum_{n=1}^N \tau \|u_h^n\|^2 dt\right)^{\frac{1}{2}} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|(\theta - \theta_h)\|^2 dt\right)^{\frac{1}{2}} \le Ch \|\theta\|_{L^2(0,T;H^1_0(\Omega))} \to 0.$$

Let us consider the next equation, that is,  $(6.1)_3$ . We have by realigning the terms,

$$\int_{0}^{T} (\mathbf{Q}_{h}^{\tau}, \psi) dt - \int_{0}^{T} (U_{h}^{\tau}, \nabla \cdot \psi) dt - \int_{0}^{T} (\mathbf{q}_{h} U_{h}^{\tau}, \psi) dt \\
= \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (\mathbf{Q}_{h}^{\tau} - \mathbf{Q}_{h}^{n}, \psi) dt + \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (\mathbf{Q}_{h}^{n}, \psi - \psi_{h}) dt \\
+ \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (u_{h}^{n} - U_{h}^{\tau}, \nabla \cdot \psi) dt + \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (U_{h}^{n}, \nabla \cdot (\psi_{h} - \psi)) dt \\
+ \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (\mathbf{q}_{h} (u_{h}^{n} - U_{h}^{\tau}), \psi) dt + \sum_{n=1}^{N} \int_{t_{n-1}}^{t_{n}} (\mathbf{q}_{h} u_{h}^{n}, \psi_{h} - \psi) dt$$
(6.30)

for all  $\psi \in L^2(0,T; H^2(\Omega))$  and where  $\psi_h$  is chosen as the  $\Pi_h$  projection of  $\psi$ . As before the left hand side converges to the desired limits. This is obvious except for the third term where we use the  $L^{\infty}$  and strong convergence of  $\mathbf{q}_h$ . Indeed,

$$\int_{0}^{T} (\mathbf{q}_{h} U_{h}^{\tau}, \boldsymbol{\psi}) dt = \int_{0}^{T} (\mathbf{q} U_{h}^{\tau}, \boldsymbol{\psi}) dt + \int_{0}^{T} ((\mathbf{q}_{h} - \mathbf{q}) U_{h}^{\tau}, \boldsymbol{\psi}) dt$$
(6.31)

and the first term on the right hand side passes to the desired limit. We show that the second term vanishes in the limit. Note that  $\mathbf{q}_h - \mathbf{q} \in (L^{\infty}(\Omega))^2$  and hence,  $(\mathbf{q}_h - \mathbf{q})U_h^{\tau}$  has a weak limit. Now choose  $\boldsymbol{\psi} \in L^2(0,T; (C_c^{\infty}(\Omega))^d), d = 2$  so that  $\boldsymbol{\psi} \in (L^{\infty}(\Omega))^2$ . Now

$$\|(\mathbf{q}_{h} - \mathbf{q})U_{h}^{\tau}\|_{(L^{1}(\Omega))^{2}} \leq \|\mathbf{q}_{h} - \mathbf{q}\|_{(L^{2}(\Omega))^{2}}\|U_{h}^{\tau}\|_{(L^{2}(\Omega))}$$

and use the strong convergence of  $\mathbf{q}_h$  in  $L^2$  (uniform with respect to h) to conclude that the weak limit is indeed 0.

Now we show that the right hand side of (6.30) vanishes in the limit. Let us denote the integrals by  $\mathcal{I}_i, i = 1, \ldots, 6$ . The successive terms will be treated as before. We begin with  $\mathcal{I}_1$ 

$$|\mathcal{I}_1| \le \|\boldsymbol{\psi}\|_{L^2(0,T;H^1(\Omega))} \left(\sum_{n=1}^N \tau \|\mathbf{Q}_h^n - \mathbf{Q}_h^{n-1}\|^2\right)^{\frac{1}{2}} \le C\tau^{\frac{1}{2}}$$

using bounds given in (6.8). Thus,  $\mathcal{I}_1$  goes to 0 in the limit. For  $\mathcal{I}_2$ , recalling the bound (6.6) and the projection estimate (3.2)

$$|\mathcal{I}_2| \le \left(\sum_{n=1}^N \tau \|\mathbf{Q}_h^n\|^2\right)^{\frac{1}{2}} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\psi - \psi_h\|_{L^2(\Omega)} dt\right)^{\frac{1}{2}} \le Ch \|\psi\|_{L^2(0,T;H(div,\Omega))} \to 0$$

as  $h \searrow 0$ .

Let us deal with the next term using (6.7),

$$|\mathcal{I}_{3}| \leq \left(\sum_{n=1}^{N} \|u_{h}^{n} - u_{h}^{n-1}\|^{2}\right)^{\frac{1}{2}} \left(\int_{0}^{T} \|\nabla \cdot \psi\|^{2} dt\right)^{\frac{1}{2}} \leq C\tau$$

which vanishes in the limit  $\tau \searrow 0$ . For  $\mathcal{I}_4$ , we have

$$|\mathcal{I}_4| \le \left(\sum_{n=1}^N \tau \|u_h^n\|^2\right)^{\frac{1}{2}} \left(\sum_{n=1}^N \int_{t_{n-1}}^{t_n} \|\nabla \cdot (\psi - \psi_h)\|^2 dt\right)^{\frac{1}{2}}$$

and further by using (6.7) and (3.2),

$$|\mathcal{I}_4| \le Ch \|\boldsymbol{\psi}\|_{L^2(0,T;H^1(\Omega))}$$

which tends to 0 as  $h \searrow 0$ . To proceed,

$$|\mathcal{I}_5| \le M_q \left( \sum_{n=1}^N \tau \|u_h^n - u_h^{n-1}\|^2 \right)^{\frac{1}{2}} \|\psi\|_{L^2(0,T;L^2(\Omega))} \le C\tau$$

with similar conclusion. Finally,

$$|\mathcal{I}_6| \le M_q \left(\sum_{n=1}^N \tau ||u_h^n||^2\right)^{\frac{1}{2}} \left(\sum_{n=1}^N \tau ||(\psi - \psi_h)||^2\right)^{\frac{1}{2}}$$

with vanishing limit due to the projection estimate (3.2) and by (6.3).

The identification of w with H(v) is identical to the semi-discrete case.

Note that the limit quadruple  $(u, \mathbf{Q}, v, w)$  indeed satisfies (4.1), but for test functions having a better regularity in space:  $\phi \in L^2(0, T; H^1_0(\Omega)), \theta \in L^2(0, T; H^1_0(\Omega))$  and  $\psi \in L^2(0, T; H^2(\Omega))$ . In view of the regularity of  $u, v, \mathbf{Q}$ , density arguments can be employed to show that the limit equations also hold for  $\phi \in L^2(0, T; L^2(\Omega)), \theta \in L^2(0, T; L^2(\Omega)), \psi \in L^2(0, T; H(div, \Omega))$ , which completes the proof.  $\Box$ 

7. Numerical computations. We consider a test problem similar to (2.1)-(2.2), but including a right hand side in the first equation (see [25] where we first announced part of these results). This is chosen in such a way that the problem has an exact solution, which is used then to test the convergence of the mixed finite element scheme. Specifically, for T = 1 and  $\Omega = (0,5) \times (0,1)$ , and with  $r(u) = [u]_{+}^{2}$  (where  $[u]_{+} := \max\{0, u\}$ ), we consider the problem

$$\begin{cases} \partial_t (u+v) + \nabla \cdot (\mathbf{q}u - \nabla u) &= f, & \text{in } \Omega^T, \\ \partial_t v &= (r(u) - w), & \text{on } \Omega^T, \\ w &\in H(v), & \text{on } \Omega^T. \end{cases}$$

Here  $\mathbf{q} = (1,0)$  is a constant velocity, whereas

$$f(t,x,y) = \frac{1}{2}e^{x-t-5} \left(1 - e^{x-t-5}\right)^{-\frac{3}{2}} \left(1 - \frac{1}{2}e^{x-t-5}\right) - \begin{cases} 0, & \text{if } x < t, \\ e^{x-t-5}, & \text{if } x \ge t, \end{cases}$$

and the boundary and initial conditions are such that

$$u(t, x, y) = (1 - e^{x - t - 5})^{\frac{1}{2}} \quad \text{and} \quad v(t, x, y) = \begin{cases} 0, & \text{if } x < t, \\ \frac{e^{x - t} - 1}{e^5} & \text{if } x \ge t, \end{cases}$$
  
providing  $w(t, x, y) = \begin{cases} 1, & \text{if } x < t, \\ 1 - e^{x - t - 5} & \text{if } x \ge t, \end{cases}$ 

form a solution triple.

We consider the mixed finite element discretization of the problem above, based on the time stepping in Section 6 and the lowest order Raviart-Thomas elements  $RT_0$ . The numerical scheme was implemented in the software package ug [6]. The simulations are carried out for a constant mesh diameter h and time step  $\tau$ , satisfying  $\tau = h$ . Further, we take  $\delta = \sqrt{h}$  as regularizing parameter. We start with h = 0.2, and refine the mesh (and correspondingly  $\tau$  and  $\delta$ ) four times successively by halving h up to h = 0.0125. We compute the errors for u and v in the  $L^2$  norms,

$$E_u^h = \|u - U^{\tau}\|_{L^2(\Omega^T)}, \text{ respectively } E_v^h = \|v - V^{\tau}\|_{L^2(\Omega^T)}$$

These are presented in Table 7.1. Although theoretically no error estimates could be given due to the particular character of the dissolution rate, Table 7.1 also includes an estimate of the convergence order, based on the reduction factor between two successive calculations:

$$\alpha = \log_2(E_u^h/E_u^{\frac{h}{2}}), \quad \text{and} \quad \beta = \log_2(E_v^h/E_v^{\frac{h}{2}}).$$

For this simple test case, the method converges linearly.

h	$\ u - U^{\tau}\ $	$\alpha$	$\ v - V^{\tau}\ $	$\beta$		
0.2	1.1700e-01		1.8409e-01			
0.1	6.414e-02	0.87	9.927e-02	0.89		
0.05	3.396e-02	0.91	5.317e-02	0.90		
0.025	1.726e-02	0.98	2.785e-02	0.93		
0.0125	8.42e-03	1.03	1.420e-02	0.97		
TABLE 7.1						

Convergence results for the mixed discretization, with explicit for v;  $h = \tau$  and  $\delta = \sqrt{\tau}$ .

A natural question is to investigate the case when we take the implicit discretization for v. This leads to a set of coupled nonlinear equation for the triple  $(u_h^n, \mathbf{Q}_h^n, v_h^n)$ . Newton's iteration is used to solve the resulting system (see [36, 40] where Newton method is applied to similar problems). We consider this case for the numerical experiments and the results are tabulated in Table 7.2. We see that for the test problem, we obtain a linear convergence rate.

h	$\ u - U^{\tau}\ $	$\alpha$	$\ v - V^{\tau}\ $	$\beta$		
0.2	1.031e-01		1.593e-01			
0.1	5.925e-02	0.79	9.023e-02	0.82		
0.05	3.247e-02	0.87	5.031e-02	0.84		
0.025	1.686e-02	0.95	2.703e-02	0.90		
0.0125	8.313e-03	1.02	1.3980e-02	0.95		
TABLE 7.2						

Convergence results for the mixed discretization, with implicit for v;  $h = \tau$  and  $\delta = \sqrt{\tau}$ .

8. Conclusions. We have considered the semi-discrete and fully discrete numerical methods for the upscaled equations. These equations describe the transport and reactions of the solutes. The numerical methods are based on mixed variational formulation where we have a separate equation for the flux. These numerical methods retain the local mass conservation property. The reaction terms are nonlinear and the dissolution term is multi-valued described by Heaviside graph. To avoid dealing with the inclusions, we use the regularized Heaviside function with the regularization parameter  $\delta$  dependent on the time step  $\tau$ . This implies that in the limit of vanishing discretization parameters automatically yields  $\delta \searrow 0$ . For the fully discrete situation, we have used mixed finite element method. The convergence analysis of both formulations have been proved using the compactness arguments, in particular the translation estimates. The proof for the fully discrete situation mirrors the proof for the semi-discrete situation however, there are important differences especially dealing with the translation estimates where we use discrete  $H_0^1$  norm to obtain compactness.

The work is complemented by the numerical experiments where we study a test case where we compare the numerical solution to the exact solution. The study provides us convergence rates for the problem studied here.

Acknowledgement. The work of K. Kumar was supported by STW project 07796. This support is gratefully acknowledged. The authors are members of the International Research Training Group NUPUS funded by the German Research Foundation DFG (GRK 1398) and by the Netherlands Organisation for Scientific Research NWO (DN 81-754). Part of the work was completed when K. Kumar visited the Institute of Mathematics, University of Bergen.

#### Numerical Analysis

#### REFERENCES

- G. Allaire, R. Brizzi, and A. Mikelić. Two-scale expansion with drift approach to the Taylor dispersion for reactive transport through porous media. *Chemical Engineering Science*, 65:2292–2300, 2010.
- T. Arbogast, M. Obeyesekere, and M. F. Wheeler. Numerical methods for the simulation of flow in root-soil systems. SIAM J. Numer. Anal., 30(6):1677–1702, 1993.
- [3] T. Arbogast and M. F. Wheeler. A characteristics-mixed finite element method for advection-dominated transport problems. SIAM J. Numer. Anal., 32(2):404–424, 1995.
- [4] J. W. Barrett and P. Knabner. Finite element approximation of the transport of reactive solutes in porous media. I. Error estimates for nonequilibrium adsorption processes. SIAM J. Numer. Anal., 34(1):201–227, 1997.
- [5] J. W. Barrett and P. Knabner. Finite element approximation of the transport of reactive solutes in porous media. II. Error estimates for equilibrium adsorption processes. SIAM J. Numer. Anal., 34(2):455–479, 1997.
- [6] P. Bastian, K. Birken, K. Johannsen, S. Lang, N. Neuss, H. Rentz-Reichert, and C. Wieners. UG a flexible software toolbox for solving partial differential equations. *Comput. and Vis. in Science*, 1:27–40, 1997.
- [7] N. Bouillard, R. Eymard, R. Herbin, and P. Montarnal. Diffusion with dissolution and precipitation in a porous medium: mathematical analysis and numerical approximation of a simplified model. M2AN Math. Model. Numer. Anal., 41(6):975–1000, 2007.
- [8] H. Brezis. Analyse fonctionnelle. Collection Mathématiques Appliquées pour la Maîtrise. [Collection of Applied Mathematics for the Master's Degree]. Masson, Paris, 1983. Théorie et applications. [Theory and applications].
- [9] F. Brezzi and M. Fortin. Mixed and hybrid finite element methods, volume 15 of Springer Series in Computational Mathematics. Springer-Verlag, New York, 1991.
- [10] E. Cariaga, F. Concha, I. S. Pop, and M. Sepúlveda. Convergence analysis of a vertex-centered finite volume scheme for a copper heap leaching model. *Math. Methods Appl. Sci.*, 33(9):1059–1077, 2010.
- [11] C. Dawson. Analysis of an upwind-mixed finite element method for nonlinear contaminant transport equations. SIAM J. Numer. Anal., 35(5):1709–1724, 1998.
- [12] C. Dawson and V. Aizinger. Upwind-mixed methods for transport equations. Comput. Geosci., 3(2):93–110, 1999.
- [13] C. N. Dawson, C. J. van Duijn, and M. F. Wheeler. Characteristic-Galerkin methods for contaminant transport with nonequilibrium adsorption kinetics. SIAM J. Numer. Anal., 31(4):982–999, 1994.
- [14] V. M. Devigne, I. S. Pop, C. J. van Duijn, and T. Clopeau. A numerical scheme for the pore-scale simulation of crystal dissolution and precipitation in porous media. SIAM J. Numer. Anal., 46(2):895–919, 2008.
- [15] C. J. van Duijn and P. Knabner. Solute transport through porous media with slow adsorption. In Free boundary problems: theory and applications, Vol. I (Irsee, 1987), volume 185 of Pitman Res. Notes Math. Ser., pages 375–388. Longman Sci. Tech., Harlow, 1990.
- [16] C. J. van Duijn and P. Knabner. Solute transport in porous media with equilibrium and nonequilibrium multiple-site adsorption: travelling waves. J. Reine Angew. Math., 415:1–49, 1991.
- [17] C. J. van Duijn and P. Knabner. Travelling wave behaviour of crystal dissolution in porous media flow. European J. Appl. Math., 8(1):49–72, 1997.
- [18] C. J. van Duijn and I. S. Pop. Crystal dissolution and precipitation in porous media: pore scale analysis. J. Reine Angew. Math., 577:171–211, 2004.
- [19] R. Eymard, T. Gallouët, and R. Herbin. Convergence of finite volume schemes for semilinear convection diffusion equations. Numer. Math., 82(1):91–116, 1999.
- [20] R. Eymard, D. Hilhorst, and M. Vohralík. A combined finite volume–nonconforming/mixed-hybrid finite element scheme for degenerate parabolic problems. *Numer. Math.*, 105(1):73–131, 2006.
- [21] D. Hilhorst and M. Vohralík. A posteriori error estimates for combined finite volume-finite element discretizations of reactive transport equations on nonmatching grids. *Comput. Methods Appl. Mech. Engrg.*, 200(5-8):597–613, 2011.
- [22] R. Klöfkorn, D. Kröner, and M. Ohlberger. Local adaptive methods for convection dominated problems. Internat. J. Numer. Methods Fluids, 40(1-2):79–91, 2002. ICFD Conference on Numerical Methods for Fluid Dynamics (Oxford, 2001).
- [23] P. Knabner, C. J. van Duijn, and S. Hengst. An analysis of crystal dissolution fronts in flows through porous media. part 1: Compatible boundary conditions. Adv. Water Resour., 18:171–185, 1995.
- [24] K. Kumar, T. L. van Noorden, and I. S. Pop. Effective dispersion equations for reactive flows involving free boundaries at the microscale. *Multiscale Model. Simul.*, 9(1):29–58, 2011.
- [25] K. Kumar, I. S. Pop, and F. A. Radu. A numerical analysis for the upscaled equations describing dissolution and precipitation in porous media. *Enumath Proceedings Volume*, 2011.
- [26] K. Kumar, I. S. Pop, and F. A. Radu. Convergence analysis for a conformal discretization of a model for precipitation and dissolution in porous media. CASA Report 12-08, Eindhoven University of Technology, 2012.
- [27] I. Metzmacher, F. A. Radu, M. Bause, P. Knabner, and W. Friess. A model describing the effect of enzymatic degradation on drug release from collagen minirods. *European Journal of Pharmaceutics and Biopharmaceutics*, 67(2):349—360, 2007.
- [28] A. Mikelić and C. J. van Duijn. Rigorous derivation of a hyperbolic model for Taylor dispersion. CASA Report 09-36, 2009.

#### Kumar, Pop, and Radu

- [29] P. Moszkowicz, J. Pousin, and F. Sanchez. Diffusion and dissolution in a reactive porous medium: mathematical modelling and numerical simulations. In Proceedings of the Sixth International Congress on Computational and Applied Mathematics (Leuven, 1994), volume 66, pages 377–389, 1996.
- [30] T. L. van Noorden. Crystal precipitation and dissolution in a thin strip. European J. Appl. Math., 20(1):69–91, 2009
- [31] T. L. van Noorden, I. S. Pop, and M. Röger. Crystal dissolution and precipitation in porous media:  $L^{1}$ contraction and uniqueness. Discrete Contin. Dyn. Syst., (Dynamical Systems and Differential Equations. Proceedings of the 6th AIMS International Conference, suppl.):1013-1020, 2007.
- [32] M. Ohlberger and C. Rohde. Adaptive finite volume approximations for weakly coupled convection dominated parabolic systems. IMA J. Numer. Anal., 22(2):253-280, 2002.
- [33] A. Pawell and K.-D. Krannich. Dissolution effects in transport in porous media. SIAM J. Appl. Math., 56(1):89-118, 1996.
- [34] J. Pousin. Infinitely fast kinetics for dissolution and diffusion in open reactive systems. Nonlinear Anal., 39(3, Ser. A: Theory Methods):261-279, 2000.
- [35] A. Quarteroni and A. Valli. Numerical approximation of partial differential equations, volume 23 of Springer Series in Computational Mathematics. Springer-Verlag, Berlin, 1994.
- [36] F. A. Radu and I. S. Pop. Newton method for reactive solute transport with equilibrium sorption in porous media. J. Comput. Appl. Math., 234(7):2118-2127, 2010.
- [37] F. A. Radu, I. S. Pop, and S. Attinger. Analysis of an Euler implicit-mixed finite element scheme for reactive solute transport in porous media. Numer. Methods Partial Differential Equations, 26(2):320-344, 2010.
- [38] F. A. Radu, I. S. Pop, and P. Knabner. Error estimates for a mixed finite element discretization of some degenerate parabolic equations. Numer. Math., 109(2):285-311, 2008.
- [39] F. A. Radu and I.S. Pop. Mixed finite element discretization and newton iteration for a reactive contaminant transport model with nonequilibrium sorption: convergence analysis and error estimates. Comput. Geosci., 15, 2011.
- [40] B. Rivière and M. F. Wheeler. Non conforming methods for transport with nonlinear reaction. In Fluid flow and transport in porous media: mathematical and numerical treatment (South Hadley, MA, 2001), volume 295 of Contemp. Math., pages 421-432. Amer. Math. Soc., Providence, RI, 2002.
- [41] J. Rubin. Transport of reacting solutes in porous media: Relation between mathematical nature of problem formulation and chemical nature of reaction. Water Resources Research, 19:1231–1252, 1983.
- [42] R. Temam. Navier-Stokes equations, volume 2 of Studies in Mathematics and its Applications. North-Holland Publishing Co., Amsterdam, third edition, 1984. Theory and numerical analysis, With an appendix by F. Thomasset.

### Appendix A. Existence of solution for $\mathbf{P}_{\delta}^{mvf,n}$ .

In this Appendix, we prove the existence of a solution for Problem  $\mathbf{P}_{\delta}^{mvf,n}$ . In this respect we keep  $\tau$  and  $\delta$  fixed and let  $h \searrow 0$  in the fully discrete problem  $\mathbf{P}_{h}^{n}$ . The limit will solve Problem  $\mathbf{P}_{\delta}^{mvf,n}$ . All the steps are similar to the fully discrete case discussed before, therefore, we only give the outline of the proof. Along a sequence  $h \searrow 0$ , Lemma 6.2 provides the following convergence results:

- 1.  $u_h^n \rightarrow u_{\delta}^n$  weakly in  $L^2(\Omega)$ , 2.  $\mathbf{Q}_h^n \rightarrow \mathbf{Q}_{\delta}^n$  weakly in  $L^2(\Omega)^d$ , 3.  $\nabla \cdot \mathbf{Q}_h^n \rightarrow \chi$  weakly in  $L^2(\Omega)$ ,
- 4.  $v_h^n \rightarrow v_\delta^n$  weakly in  $L^2(\Omega)$ .

As before, identification of  $\chi$  with  $\nabla \cdot \mathbf{Q}_{\delta}^{n}$  takes place via standard arguments. Further, Lemma 6.6 with the estimates (6.3) and (6.6) gives

 $||u_h^n||_{1,h} \le C$ 

and after extending  $u_h^n$  by 0, Lemma 6.5 implies

$$\|\triangle_{\xi} u_h^n\|_{L^2(\mathbb{R}^2)} \le C|\xi|(|\xi| + \operatorname{size}(\mathcal{T}_h)).$$

Since the right hand side vanishes uniformly as  $|\xi| \searrow 0$ , the use of Kolmogorov compactness theorem yields strong convergence of  $u_h^n$  to  $u_{\delta}^n$ . Now one can use the projection properties and pass  $h \searrow 0$  to show that the limit solves  $\mathbf{P}_{\delta}^{mvf,n}$ . Note that having v discretized explicitly in  $(6.1)_2$ , no nonlinearities in  $v_h^n$  are involved and therefore there is no need for strong convergence for  $v_h^n$ .

## PREVIOUS PUBLICATIONS IN THIS SERIES:

Number	Author(s)	Title	Month
12-16	O. Matveichuk J.J.M. Slot	A rod-spring model for main-chain liquid crystalline polymers containing hairpins	May '12
12-17	T. Doorn E.J.W. ter Maten A. Di Bucchianico T. Beelen R. Janssen	Access time optimization of SRAM memory with statistical yield constraint	May '12
12-18	E.R. IJioma T. Ogawa A. Muntean	Pattern formation in revers smoldering combustion: A homogenization approach	May '12
12-19	C. Mercuri F. Pacella	On the pure critical exponent problem for the p-Laplacian	May '12
I2-20	K. Kumar I.S. Pop F.A. Radu	Convergence analysis of mixed numerical schemes for reactive flow in a porous medium	June '12
			Ontwerp: de Tantes, Tobias Baanders, CWI