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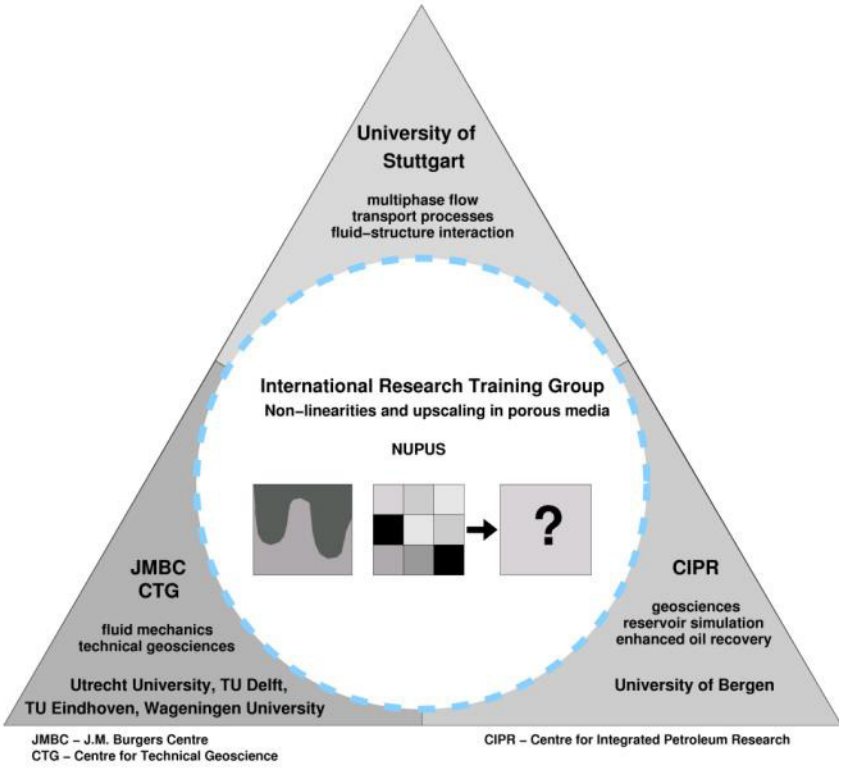

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Analysis and upscaling of a reactive transport model in fractured porous media involving nonlinear a transmission condition

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Abstract We consider a reactive transport model in a fractured porous medium. The particularity appears in the conditions imposed at the interface separating the block and the fracture, which involves a nonlinear transmission condition. Assuming that the fracture has thickness ε, we analyze the resulting problem and prove the convergence towards a *reduced* model in the limit $\varepsilon \searrow 0$. The resulting is a model defined on an interface (the reduced fracture) and acting as a boundary condition for the equations defined in the block. Using both formal and rigorous arguments, we obtain the reduced models for different flow regimes, expressed through a moderate, or a high Peclét number.

Keywords Fractured porous media · Upscaling · Reactive transport · Nonlinear transmission conditions

1 Introduction

Fractures are ubiquitous in porous media and have strong influence on the flow and transport. Several energy and environmental applications including carbon sequestration, geothermal energy, hydraulic fracturing, petroleum extraction, or ground water contamination, are involving flow and reactive transport in fractured porous media. Typically, fractures are thin and long formations along which medium properties like permeability, or porosity, are different from the adjacent formations (the blocks). This leads to media with high contrasting properties appearing in anisotropic regions, and involving jump-type discontinuities across interfaces between the fracture and the block. This makes the

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numerical simulation of mathematical models in such domains a very challenging task. Discretization schemes resolving the full thin fracture regions explicitly is prohibitively expensive. Moreover, often the main interest is in the transport or flow along fractures and not in the transverse details. This suggests considering the so called *reduced models* for the processes inside fractures, which are transversally averaged along such formations, and reduce the fracture itself to an interface separating two blocks. The resulting problem is defined in a bulk domain (the union of the porous blocks), as well as on surfaces (the lower dimensional approximation of the fractures) embedded in the bulk domain. Nevertheless, the surface should incorporate the averaged processes in the fracture, including the coupling conditions between the fracture and the adjacent blocks. This requires a consistent procedure for developing such reduced models.

In this work, both formal and rigorous procedures are used for deriving reduced models that describe reactive transport in fractured media. The flow is assumed to be known in the thin fractures, and the transport is modelled by a convection-diffusion equation. Inside blocks, which are typically less permeable than fractures, no flow is encountered, and species undergo only diffusive transport. The particularity of the model lies in the conditions coupling the models inside fractures and blocks at the common interface. Next to the normal flux continuity, a nonlinear transmission condition is imposed. For the ease of presentation, we consider a simple geometry, where a large rectangular domain (the porous block) is coupled to a rectangular fracture with small thickness ε. After transversal averaging in the fracture and letting ε go to zero, the fracture model becomes a boundary condition for the partial differential equation in the bulk domain. This procedure is carried out formally in two situations, when the flow and transport processes in the fracture are in balance (moderate Peclét regime), and when flow is dominating (high Peclét regime). Then, convergence is obtained rigorously for the moderate Peclét regime.

Reactive transport in heterogeneous media lead naturally to nonlinear transmission conditions. Examples in this sense appear in bubble columns or extraction processes involving multiphase systems. In ionic fluids, which are strongly non-ideal, nonlinear reactions are encountered at interfaces separating two domains [33]. Well-known examples in this sense are Langmuir, Freundlich or Monod type reactions. Such models are also the outcome of the upscaling procedure in [20,26,27,28,29]. Nonlinear transmission conditions also appear in multiphase flow models in porous media [10], where e.g. pressure continuity at interface separating a fine and a coarse porous block induces a nonlinear relation between the oil saturations at the two sides of the interface.

Due to their high permeability in the fractures one encounters both convection and diffusion processes. Related, at least two different time scales can be identified: a convective time scale T_C, and a diffusive one T_D. Their ratio defines the non-dimensional Peclét number, $Pe = \frac{T_D}{T_C}$. The observed transport behaviour depends strongly on this number, in particular, when the convection dominates (high Peclét), the net diffusion is enhanced by the convective

strength itself exhibiting the well-known Taylor dispersion [34,19,25]. The upscaling procedure needs to take these complexities into account.

The results in this paper are the following. For a fixed ε, the existence of solutions for the system involving two parabolic models posed in adjacent domains, and involving a nonlinear transmission conditions is proved. This is obtained by Rothe's method [16] and essentially uses the existence results for elliptic problems obtained in [14]. We also mention that the full model (i.e. when $\varepsilon > 0$) considered here is similar to the one in [15]. Here the existence results are obtained directly for the original unknowns, and without employing a nonlinear transformation of these in order to obtain the continuity across the interface. This is closer to the approaches in [6,7,23] and allows extending the present results to the case of heterogeneous (e.g. spatially dependent) transmission conditions. Next, we derive the reduced models by averaging in the transversal direction of the fracture, and using formal asymptotic methods. This is achieved for two regimes in the fracture, moderate Péclet, $Pe = \mathcal{O}(1)$, and transport dominated regime $Pe = \mathcal{O}(\varepsilon^{-1})$. Finally, for the case when $Pe = \mathcal{O}(1)$, we rigorously prove convergence of the full model, including the nonlinear transmission condition, to the simple, upscaled model obtained by formal asymptotics.

The paper is structured as follows. In Section 2, we introduce the mathematical model and in Section 3 we prove the existence of a solution for a fixed ε with the necessary a priori estimates derived in Section 3.4. Next, we perform a formal upscaling for both moderate and high Peclét number in sections 4 and 4.2, respectively. Section 5 deals with rigorous derivation of the upscaled equations obtained in Section 4. Full details can be found in [4], Chapters 4, 5 and 9. The paper concludes with discussions and outlook in Section 6.

2 Model and assumptions

The problem is stated in a dimensionless framework and we refer e.g. to [9,11, 19] for a non-dimensionalization step. Let $T > 0$ be a maximal time and Ω_p (the porous block) and Ω_f^ε (the fracture) be two adjacent domains separated by the interface Γ:

$$\begin{aligned}
\Omega_p &:= \{(x,y) \in \mathbb{R}^2 | 0 < x < 1, -1 < y < 0\},\\
\Omega_f^\varepsilon &:= \{(x,y) \in \mathbb{R}^2 | 0 < x < 1, 0 < y < \varepsilon\},\\
\Gamma &:= \{(x,y) \in \mathbb{R}^2 | 0 < x < 1, y = 0\},\\
\Gamma_{f,1}^\varepsilon &:= \{(x,y) \in \mathbb{R}^2 | x = 0, 0 < y < \varepsilon\},\\
\Gamma_{f,3}^\varepsilon &:= \{(x,y) \in \mathbb{R}^2 | x = 1, 0 < y < \varepsilon\},\\
\Gamma_{p,1} &:= \{(x,y) \in \mathbb{R}^2 | x = 0, -1 < y < 0\},\\
\Gamma_{p,3} &:= \{(x,y) \in \mathbb{R}^2 | x = 1, -1 < y < 0\},\\
\Gamma_{p,2} &:= \{(x,y) \in \mathbb{R}^2 | 0 < x < 1, y = -1\},\\
\Gamma_{f,2}^\varepsilon &:= \{(x,y) \in \mathbb{R}^2 | 0 < x < 1, y = \varepsilon\}.
\end{aligned} \tag{1}$$

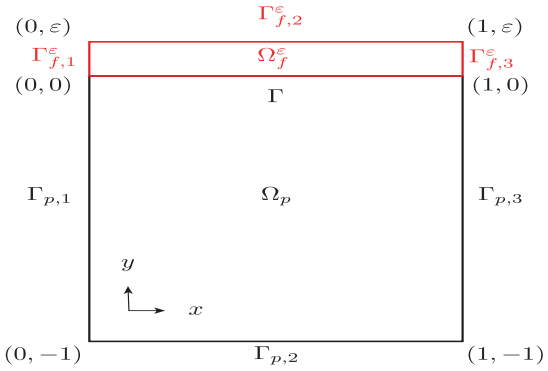

Fig. 1 Geometry depicting a fracture coupled to an adjacent porous medium. The fracture is of thickness 2ε, and due to symmetry it is sufficient to consider only half of the fracture. $\Gamma_{f,2}^{\varepsilon}$ is this line of symmetry.

The remaining boundaries of Ω_p and Ω_f are $\Gamma_{p,\imath}$, respectively $\Gamma_{f,\imath}$ ($\imath = 1,2,3$), see Figure 1. Here $\varepsilon > 0$ is the half-fracture aperture (because of symmetry) and is assumed small compared to the fracture length.

2.1 Notation

Before stating the model, we mention that standard notations from the functional analysis are being used below. By $(\cdot,\cdot)$ we mean L^2 inner product or the duality pairing between $W^{1,2}$ and its dual. By $Tr(\cdot)$ we denote the trace operator. Further, with X being a Banach space, $C(0,T;X)$ stands for the X-valued functions that are continuous over $[0,T]$, and $L^p(0,T;X)$ is the usual Bochner space. Next, for the weak solutions we will use the spaces

$$V_p := \{u \in W^{1,2}(\Omega_p) | u = 0 \text{ on } \Gamma_{p,1} \cup \Gamma_{p,3}\}, \tag{2}$$

$$V_f^{\varepsilon} := \{u \in W^{1,2}(\Omega_f^{\varepsilon}) | u = 0 \text{ on } \Gamma_{f,1}^{\varepsilon} \cup \Gamma_{f,3}^{\varepsilon}\}, \tag{3}$$

with $\Gamma_{p,1}$,$\Gamma_{p,3}$, $\Gamma_{f,1}^{\varepsilon}$ and $\Gamma_{f,3}^{\varepsilon}$ defined in (1). Since V_p is a closed subspace of the Hilbert space $W^{1,2}(\Omega_p)$, it is again a Hilbert space, equipped with the $W^{1,2}(\Omega_p)$ norm and inner product. Similarly, V_f^{ε} is a Hilbert space equipped with the $W^{1,2}(\Omega_f^{\varepsilon})$ norm and inner product. For $u \in L^2(0,T;V_p^*)$ and $v \in L^2(0,T;V_p)$, we define

$$(u,v)_{\Omega_p^T} := \int_0^T \langle u(t), v(t)\rangle_{\Omega_p} dt, \text{ where } \langle u(t), v(t)\rangle_{\Omega_p} := \langle u(t), v(t)\rangle_{V_p^*, V_p}.$$

The counterparts for the fracture domains are defined similarly. Finally, let

$$\mathcal{W}_p := \{u \in L^2(0,T;V_p) \big| \partial_t u \in L^2(0,T;V_p^*)\}, \tag{4}$$

$$\mathcal{W}_f^{\varepsilon} := \{u \in L^2(0,T;V_f^{\varepsilon}) \big| \partial_t u \in L^2(0,T;(V_f^{\varepsilon})^*)\}. \tag{5}$$

We observe that, by Assumption A_r below, if $u \in W^{1,2}(\Omega)$, then $r(u) \in W^{1,2}(\Omega)$ as well, and hence $Tr(r(u))$ is well defined, belonging to $L^2(\partial\Omega)$.

2.2 Mathematical model

The unknown quantities are the concentrations $u_p^\varepsilon, u_f^\varepsilon$ of two chemical species defined in Ω_p and Ω_f^ε, respectively. The transporting mechanisms are diffusion in Ω_p and convection and diffusion in Ω_f^ε, respectively. The models in the two domains are coupled at Γ through two conditions: the continuity of the normal fluxes, and the nonlinear reactions (the nonlinear transmission condition). We assume symmetry along $\Gamma_{f,2}^\varepsilon$. This is summarized in:

$$\begin{cases} \partial_t u_p^\varepsilon - \Delta u_p^\varepsilon = f_p, & \text{in } (0,T]\times\Omega_p, \\ \partial_t u_f^\varepsilon + \mathbf{q}^\varepsilon\cdot\nabla u_f^\varepsilon - \Delta u_f^\varepsilon = f_f, & \text{in } (0,T]\times\Omega_f^\varepsilon, \\ u_f^\varepsilon = r(u_p^\varepsilon), & \text{at } (0,T]\times\Gamma, \\ \partial_{\boldsymbol{\nu}} u_p^\varepsilon = \partial_{\boldsymbol{\nu}} u_f^\varepsilon, & \text{at } (0,T]\times\Gamma. \end{cases} \tag{6}$$

Boundary and initial conditions are specified below. Here the diffusion coefficients are taken exactly 1, but extending the presentation to more general coefficients D_p and D_f, or positive definite tensors, is immediate. In Section 4, where formal upscaling will be carried out, we consider an ε order diffusion in the fracture as well to include the convection dominated regime. f_p and f_f^ε are source terms, and $\mathbf{q}^\varepsilon$ is a given fluid velocity, all satisfying assumptions mentioned below.

2.3 Assumptions

The particularity is in the nonlinear transmission conditions at Γ, involving the function r. For this we assume

(A_r) The function $r \in C^1(\mathbb{R})$ satisfies $r(0) = 0$, and there exist $m, M > 0$ such that for all $u \in \mathbb{R}$, $0 < m \le r'(u) \le M < \infty$.

The concentrations vanish on the vertical boundaries,

$$u_f^\varepsilon = 0, \text{ on } \Gamma_{f,1}^\varepsilon \cup \Gamma_{f,3}^\varepsilon, \text{ and } u_p^\varepsilon = 0, \text{ on } \Gamma_{p,1}\cup\Gamma_{p,3}. \tag{7}$$

Remark 1 *By Assumption A_r, r has a C^1 inverse r^{-1} satisfying*

$$0 < \frac{1}{M} \le \left(r^{-1}\right)'(u) \le \frac{1}{m} < \infty, \qquad \textit{for all } u \in \mathbb{R}.$$

This gives $0 \le \left(r^{-1}\right)(u) \le \frac{1}{m}u$ for all $u \ge 0$.

Below we will use the antiderivative of r, defined as

$$R : \mathbb{R} \to \mathbb{R}, \qquad R(u) := \int_0^u r(v)dv. \tag{8}$$

Using Assumption A_r and the Mean Value Theorem, the following can be proved straightforwardly

Proposition 2 *The function R has the following elementary properties:*
(i) $R(x) \geq 0$, for all $x \in \mathbb{R}$.
(ii) $R(y) - R(x) \leq r(y)(y-x)$, for all $x, y \in \mathbb{R}$.
(iii) $R(x) \geq \frac{m}{2}x^2$, for all $x \in \mathbb{R}$.

Further, we assume

(A_f) The functions $f_p \in C(0,T;L^2(\Omega_p))$ and $f_f \in C(0,T;L^2(\Omega_f^\varepsilon))$ are bounded and positive: there exist $M_f > 0$ such that for all $t \in [0,T]$,

$$0 \leq f_f(t,\cdot) \leq M_f \text{ a.e. in } \Omega_f^\varepsilon, \quad \text{and} \quad 0 \leq f_p(t,\cdot) \leq M_f \text{ a.e. in } \Omega_p.$$

(A_I) The initial conditions are positive and essentially bounded: there exist $M_I > 0$ such that

$$0 \leq u_{I,f} \leq M_I \text{ a.e. in } \Omega_f^\varepsilon, \quad \text{and} \quad 0 \leq u_{I,p} \leq M_I \text{ a.e. in } \Omega_p.$$

(A_q) The velocity field $\mathbf{q}^\varepsilon = (q^{\varepsilon,1}, q^{\varepsilon,2}) \in [W^{1,2}(\Omega_f^\varepsilon)]^2$ isatisfies

$$\nabla \cdot \mathbf{q}^\varepsilon = 0 \text{ in } \Omega_f^\varepsilon, \quad \text{and} \quad \mathbf{q}^\varepsilon = \mathbf{0} \text{ on } \Gamma.$$

Further, $q^{\varepsilon,2} = 0$ at $\Gamma_{f,2}^\varepsilon$ (symmetry). Finally, $\mathbf{q}^\varepsilon$ is essentially bounded: there exists $M_q > 0$ s.t. $||\mathbf{q}^\varepsilon|| \leq M_q$ a.e. in Ω_f^ε.

Concerning A_q, this holds true if e.g., $\mathbf{q}$ solves the Stokes model with homogeneous Dirichlet boundary conditions, see [17,21]. To simplify the calculations, the initial data are assumed ε-independent, i.e. $u_p^\varepsilon(0,x,y) = u_{I,p}(x,y)$ and $u_f^\varepsilon(0,x,y) = u_{I,f}(x)$. Similarly, the source terms are ε-independent too.

3 Existence of a weak solution

We first prove the existence of a weak solution for the original model in (6), with the initial and boundary conditions stated above. This is defined in

Definition 3 *A pair $(u_f, u_p) \in L^2(0,T;V_f^\varepsilon) \times L^2(0,T;V_p)$ is called a weak solution of (6) if $u_f = r(u_p)$ on Γ (in the sense of traces) and*

$$\begin{aligned} &-(u_f, \partial_t \phi_f)_{\Omega_f^{\varepsilon,T}} - (u_p, \partial_t \phi_p)_{\Omega_p^T} + (\mathbf{q}\cdot\nabla u_f, \phi_f)_{\Omega_f^{\varepsilon,T}} \\ &+ (\nabla u_f, \nabla \phi_f)_{\Omega_f^{\varepsilon,T}} + (\nabla u_p, \nabla \phi_p)_{\Omega_p^T} \\ =&(f_f, \phi_f)_{\Omega_f^T} + (f_p, \phi_p)_{\Omega_p^T} + (u_{I,f}, \phi_f(0))_{\Omega_f^\varepsilon} + (u_{I,p}, \phi_p(0))_{\Omega_p}, \end{aligned} \tag{9}$$

for all $(\phi_f, \phi_p) \in W^{1,2}(0,T;V_f^\varepsilon) \times W^{1,2}(0,T;V_p)$ such that $\phi_f = \phi_p$ on Γ and $\phi_f(T) = \phi_p(T) = 0$.

The existence of a weak solution is obtained by the Rothe's method [16]. In doing so, the ε dependence in the a-priori estimates is stated explicitly.

3.1 Discretization in time

Letting Δt be a fixed time step, taking $u_i^0 = u_{I,i}$ ($i \in \{f,p\}$), we construct the Euler implicit approximations $\{u_i^k\}_{k\in\mathbb{N}}$ of u_i at $t_k = k\Delta t$. This leads to a sequence of elliptic problems involving again a nonlinear transmission condition. We omit the strong form here and provide directly the definition of a weak solution, which is stated in

Definition 4 *Let $k > 0$ and let $(u_f^{k-1}, u_p^{k-1}) \in V_f^\varepsilon \times V_p$ be given. A weak solution to the time discrete problem at t_k is a pair $(u_f^k, u_p^k) \in V_f^\varepsilon \times V_p$ satisfying $u_f^k = r(u_p^k)$ on Γ (in the sense of traces) and*

$$\begin{aligned}&\big(\frac{u_f^k - u_f^{k-1}}{\Delta t}, \phi_f\big)_{\Omega_f^\varepsilon} + \big(\frac{u_p^k - u_p^{k-1}}{\Delta t}, \phi_p\big)_{\Omega_p} + (\nabla u_f^k, \nabla\phi_f)_{\Omega_f^\varepsilon} + (\nabla u_p^k, \nabla\phi_p)_{\Omega_p}\\ &+ (\mathbf{q}\cdot\nabla u_f^k, \phi_f)_{\Omega_f^\varepsilon} = (f_f(t_k), \phi_f)_{\Omega_f^\varepsilon} + (f_p(t_k), \phi_p)_{\Omega_p} \qquad (10)\end{aligned}$$

for all $(\phi_f, \phi_p) \in V_f^\varepsilon \times V_p$ such that $\phi_f = \phi_p$ on Γ.

Such elliptic problems are studied in [14], where the existence and uniqueness of a weak solution is proved.

3.2 A priori estimates

We start by observing that for any $u \in V_p$, since $r \in C^1$ we have $r(u) \in V_f$ as well. This will be used below to prove

Lemma 1 *For the sequence of time discrete weak solutions in Definition 4, a $C > 0$ not depending on Δt exists s.t.*

$$\begin{aligned}&\max_{j\in\{1,\dots,N\}} \left|\left|u_f^j\right|\right|^2_{\Omega_f^\varepsilon} + \max_{j\in\{1,\dots,N\}} \int_{\Omega_p} R(u_p^j)dx\\ &+ \sum_{k=1}^N \left|\left|u_f^k - u_f^{k-1}\right|\right|^2_{\Omega_f^\varepsilon} + \Delta t \sum_{k=1}^N \left\{ \left|\left|\nabla u_f^k\right|\right|^2_{\Omega_f^\varepsilon} + \left|\left|\nabla u_p^k\right|\right|^2_{\Omega_p} \right\} \le C. \qquad (11)\end{aligned}$$

Proof We test with $\phi_f := u_f^k$ and $\phi_p := r(u_p^k)$ in (10) and denote the resulting terms by $I_1, I_2, ..., I_7$. Clearly,

$$I_1 = \frac{1}{2}\left|\left|u_f^k\right|\right|^2_{\Omega_f^\varepsilon} + \frac{1}{2}\left|\left|u_f^k - u_f^{k-1}\right|\right|^2_{\Omega_f^\varepsilon} - \frac{1}{2}\left|\left|u_f^{k-1}\right|\right|^2_{\Omega_f^\varepsilon}.$$

To treat I_2, we use Proposition 2 to obtain

$$I_2 \ge \int_{\Omega_p} R(u_p^k)dx - \int_{\Omega_p} R(u_p^{k-1})dx.$$

Note that, since R is positive, $\int_{\Omega_p} R(u_p^k)dx \ge 0$ for all $k \in \{0, ..., N\}$.

For I_3, using the Poincaré inequality gives

$$I_3 \ge \frac{1}{2}\left|\left|\nabla u_f^k\right|\right|^2_{\Omega_f^\varepsilon} + \frac{1}{2C_f}\left|\left|u_f^k\right|\right|^2_{\Omega_f^\varepsilon},$$

for a C_f depending only on the geometry of Ω_f^ε. Actually, in view of the boundary conditions on $\Gamma_{\varepsilon,1}$ and $\Gamma_{\varepsilon,3}$, the constant C_f is ε independent.

For I_4 we proceed similarly, to obtain

$$I_4 \geq m \left|\left|\nabla u_p^k\right|\right|_{\Omega_p}^2 \geq \frac{m}{2} \left|\left|\nabla u_p^k\right|\right|_{\Omega_p}^2 + \frac{m}{2C_p} \left|\left|u_p^k\right|\right|_{\Omega_p}^2,$$

where C_p depends only on the geometry of Ω_p.

The convection term I_5 vanishes. Indeed,

$$\begin{aligned}(\mathbf{q}\cdot\nabla u_f^k, u_f^k)_{\Omega_f^\varepsilon} &= (\mathbf{q}\cdot\nabla u_f^k, u_f^k)_{\Omega_f^\varepsilon} = \frac{1}{2}(\mathbf{q}, (\nabla u_f^k)^2)_{\Omega_f^\varepsilon} \\ &= \frac{1}{2}((u_f^k)^2\mathbf{q}, \boldsymbol{\nu})_{\partial\Omega_f^\varepsilon} - \frac{1}{2}((u_f^k)^2, \nabla\cdot\mathbf{q})_{\Omega_f^\varepsilon} = 0,\end{aligned}$$

by the boundary conditions on $\partial\Omega_f^\varepsilon$ and the properties of $\mathbf{q}$

Using the Cauchy-Schwarz inequality and Young's inequality gives for I_6 and I_7

$$\begin{aligned}|I_6| &\leq ||f_f(t_k)||_{\Omega_f^\varepsilon} \left|\left|u_f^k\right|\right|_{\Omega_f^\varepsilon} \leq \frac{1}{2C_f} \left|\left|u_f^k\right|\right|_{\Omega_f^\varepsilon}^2 + \frac{C_f}{2} ||f_f(t_k)||_{\Omega_f^\varepsilon}^2, \text{ and} \\ |I_7| &\leq M ||f_p(t_k)||_{\Omega_p} \left|\left|u_p^k\right|\right|_{\Omega_p} \leq M^2 \frac{C_p}{2m} ||f_p(t_k)||_{\Omega_p}^2 + \frac{m}{2C_p} \left|\left|u_p^k\right|\right|_{\Omega_p}^2.\end{aligned}$$

Using the estimates above into (10) and summing for $k = 1, ..., j$ (where $j \leq N$ is arbitrary) gives

$$\begin{aligned}&\frac{1}{2}\left|\left|u_f^j\right|\right|_{\Omega_f}^2 + \frac{1}{2}\sum_{k=1}^{j}\left|\left|u_f^k - u_f^{k-1}\right|\right|_{\Omega_f^\varepsilon}^2 + \int_{\Omega_p} R(u_p^j)dx \\ &+ \frac{\Delta t}{2}\sum_{k=1}^{j}\left|\left|\nabla u_f^k\right|\right|_{\Omega_f^\varepsilon}^2 + \frac{m\Delta t}{2}\sum_{k=1}^{j}\left|\left|\nabla u_p^k\right|\right|_{\Omega_p}^2 \\ \leq &\frac{1}{2}\left|\left|u_f^0\right|\right|_{\Omega_f^\varepsilon}^2 + \int_{\Omega_p} R(u_p^0)dx + \Delta t\frac{C_p}{2}\sum_{k=1}^{j}||f_f(t_k)||_{\Omega_f^\varepsilon}^2 + \Delta t\frac{C_pM^2}{2m}\sum_{k=1}^{j}||f_p(t_k)||_{\Omega_p}^2.\end{aligned}$$

In view of assumptions A_I and A_f, the sums on the right are bounded uniformly in Δt and j. This proves the estimates.

In a similar fashion one obtains

Lemma 2 *For the sequence of time discrete weak solutions in Definition 4, a $C > 0$ not depending on Δt exists s.t.*

$$\max_{j\in\{1,\ldots,N\}}\left|\left|u_p^j\right|\right|_{\Omega_p}^2 + \sum_{k=1}^{N}\left|\left|u_p^k - u_p^{k-1}\right|\right|_{\Omega_p}^2 \leq C. \tag{12}$$

Proof As before, $\phi_f := r^{-1}(u_f^k) \in V_f^\varepsilon$, and it can be used together with $\phi_p := u_p^k$ as test functions in (10). The proof follows as above, but involves the antiderivative R^* of r^{-1} for showing that the convection term vanishes:

$$(\mathbf{q}\cdot\nabla u_f^k, r^{-1}(u_f^k))_{\Omega_f^\varepsilon} = (\mathbf{q}, \nabla R^*(u_{\varepsilon,,f}^k))_{\Omega_f^\varepsilon},$$

and the rest follows as before.

3.3 Interpolation in time and convergence

Having obtained the a priori estimates, the time discrete pairs are used to construct piecewise linear and piecewise constant interpolations in time. More precisely, for almost every $t \in (t_{k-1}, t_k]$, we define

$$\bar{U}^f_{\Delta t}(t) := u^k_f, \quad \hat{U}^f_{\Delta t}(t) := u^{k-1}_f + \frac{t - t_{k-1}}{\Delta t}(u^k_f - u^{k-1}_f), \tag{13}$$

$$\bar{U}^p_{\Delta t}(t) := u^k_p, \quad \hat{U}^p_{\Delta t}(t) := u^{k-1}_p + \frac{t - t_{k-1}}{\Delta t}(u^k_p - u^{k-1}_p). \tag{14}$$

Further, the piecewise constant interpolation of the source terms will be used

$$\bar{f}^i_{\Delta t}(t) := f_i(t_k).$$

For the ease of writing, we take $i \in \{p, f\}$, and omit the superscript ε for the quantities, domains, or spaces involving the fracture. Using the a priori estimates in Lemmata 1 and 2, one gets for $\bar{U}^i_{\Delta t}$:

Lemma 3 *$\{\bar{U}^i_{\Delta t}\}_{\Delta t>0}$ is bounded uniformly w.r.t Δt in $L^\infty(0,T;L^2(\Omega_i)) \cap L^2(0,T;V_i)$.*

Due to the a priori bounds in Lemma 3, there exists a subsequence (along $\Delta t \searrow 0$) of the time interpolations in (13)–(14) that converges weakly in $L^2(0,T;V_f) \times L^2(0,T;V_p)$. Here we show that the weak limit is a solution in the sense of Definition 3. We start with a strong convergence result, which is needed for the convergence on the boundary Γ. In doing so, we use the following result (Lemma 3.2 in [23]).

Lemma 4 *Let X be a Hilbert space. The strong convergence*

$$\hat{U}^i_{\Delta t} \to U_i \qquad \text{in } L^2(0,T;X),$$

implies the strong convergence

$$\bar{U}^i_{\Delta t} \to U_i \qquad \text{in } L^2(0,T;X). \tag{15}$$

Based on this, we obtain the strong convergence in $L^2(0,T;L^2(\Omega_i))$.

Lemma 5 *Along a sequence $\Delta t \searrow 0$, the piecewise constant in time approximations $(\bar{U}^f_{\Delta t}, \bar{U}^p_{\Delta t})$ converge strongly in $L^2(0,T;L^2(\Omega_f)) \times L^2(0,T;L^2(\Omega_p))$.*

Proof The proof is given for the fracture ($i = f$), the arguments for $i = p$ being exactly the same. For $t \in (t_{k-1}, t_k]$ we regard $\partial_t \hat{U}_{\Delta t} = \frac{u^k_f - u^{k-1}_f}{\Delta t}$ as an element in $L^2(0,T;W^{-1,2}(\Omega_f))$, where $W^{-1,2}(\Omega_f)$ is the dual of $W^{1,2}_0(\Omega_f)$ (the $W^{1,2}(\Omega_f)$ functions having a vanishing trace over the entire $\partial\Omega_f$) identified by the duality pairing

$$\langle \partial_t \hat{U}^f_{\Delta t}(t), \phi_f \rangle_{W^{-1,2}(\Omega_f), W^{1,2}_0(\Omega_f)} = \frac{1}{\Delta t}(u^k_f - u^{k-1}_f, \phi_f)_{\Omega_f},$$

for all $\phi_f \in W_0^{1,2}(\Omega_f)$. Testing in (10) with $\phi_p \equiv 0$ and an arbitrary $\phi_f \in W_0^{1,2}(\Omega_f)$ gives

$$\langle \partial_t \hat{U}^f_{\Delta t}(t), \phi_f \rangle_{(W^{-1,2}(\Omega_f)),W_0^{1,2}(\Omega_f)} + (\nabla u_f^k, \nabla \phi_f)_{\Omega_f} + (\mathbf{q} \cdot \nabla u_f^k, \phi_f)_{\Omega_f} = (f_f(t_k), \phi_f)_{\Omega_f},$$

providing for $t \in (t_{k-1}, t_k]$

$$\left|\left|\partial_t U^f_{\Delta t}(t)\right|\right|_{W^{-1,2}(\Omega_f)} \leq (1 + M_q) \left|\left|\nabla u_f^k\right|\right|_{\Omega_f} + ||f_f(t_k)||_{\Omega_f}.$$

Here M_q is the bound on the velocity profile, as introduced in Assumption A_q. Using now the estimates in Lemma 1 an the assumptions of f_f one gets that $\partial_t U^f_{\Delta t}$ is bounded in $L^2(0,T;W^{-1,2}(\Omega_f))$ uniformly w.r.t. Δt.

By [32], the above boundedness together with the uniform boundedness of $\hat{U}^f_{\Delta t}$ in $L^2(0,T;V_f)$ provide the existence of a limit U_f s.t. along a sequence $\Delta t \searrow 0$,

$$\hat{U}^f_{\Delta t} \to U_f, \qquad \text{strongly in } L^2(0,T;L^2(\Omega_f)).$$

Further, Lemma 4 gives the strong convergence for $\bar{U}^f_{\Delta t}$ to the same limit U_f, and the proof is finished.

By Lemmata 3 and 5, a sequence Δt exists s.t.

$$\begin{array}{l} \bar{U}^f_{\Delta t} \to U_f, \text{ weakly in } L^2(0,T;V_f) \text{ and strongly in } L^2(0,T;L^2(\Omega_f)), \\ \bar{U}^p_{\Delta t} \to U_p, \text{ weakly in } L^2(0,T;V_p) \text{ and strongly in } L^2(0,T;L^2(\Omega_p)). \end{array} \tag{16}$$

We show that the limit pair is a weak solution

Theorem 5 *The pair (U_f, U_p) is a solution in the sense of Definition 3.*

Proof We start by summing (10) from $j = 1, ..., k$. Recalling (13) and (14), for any $(\phi_f, \phi_p) \in V_f \times V_p$ such that $\phi_f = \phi_p$ on Γ one gets for every $t \in (t_{k-1}, t_k)$

$$\begin{aligned} &(\bar{U}^f_{\Delta t}(t), \phi_f)_{\Omega_f} + (\bar{U}^p_{\Delta t}(t), \phi_p)_{\Omega_p} + \int_0^t (\nabla \bar{U}^f_{\Delta t}(\tau), \nabla \phi_f)_{\Omega_f} d\tau \\ &+ \int_0^t (\nabla \bar{U}^p_{\Delta t}(\tau), \nabla \phi_p)_{\Omega_p} d\tau + \int_0^t (\mathbf{q} \cdot \nabla \bar{U}^f_{\Delta t}(\tau), \phi_f)_{\Omega_f} d\tau \\ &- \int_0^t (\bar{f}_f(\tau), \phi_f)_{\Omega_f} d\tau - \int_0^t (\bar{f}_p(\tau), \phi_p)_{\Omega_p} d\tau - (u_{I,f}, \phi_f)_{\Omega_f} - (u_{I,p}, \phi_p)_{\Omega_p} \\ = &\int_t^{t_k} (\bar{f}_f(\tau), \phi_f)_{\Omega_f} d\tau + \int_t^{t_k} (\bar{f}_p(\tau), \phi_p)_{\Omega_p} d\tau - \int_t^{t_k} (\nabla \bar{U}^f_{\Delta t}(\tau), \nabla \phi_f)_{\Omega_f} d\tau \\ &- \int_t^{t_k} (\nabla \bar{U}^p_{\Delta t}(\tau), \nabla \phi_p)_{\Omega_p} d\tau - \int_t^{t_k} (\mathbf{q} \cdot \nabla \bar{U}^f_{\Delta t}(\tau), \phi_f)_{\Omega_f} d\tau, \end{aligned}$$

The terms on the right are accounting for the fact that, actually, the upper limit in the time integrals on the left should be t_k. Next, take $\phi_i \in L^2(0,T;V_i)$, such that $\phi_f = \phi_p$ on Γ, and integrate over $[0,T]$, to obtain

$$\begin{aligned}
&\int_0^T (\bar{U}^f_{\Delta t}(t), \phi_f(t))_{\Omega_f} dt + \int_0^T (\bar{U}^p_{\Delta t}(t), \phi_p(t))_{\Omega_p} dt \\
&+ \int_0^T \int_0^t (\nabla \bar{U}^f_{\Delta t}(\tau), \nabla \phi_f(t))_{\Omega_f} d\tau dt + \int_0^T \int_0^t (\nabla \bar{U}^p_{\Delta t}(\tau), \nabla \phi_p(t))_{\Omega_p} d\tau dt \\
&+ \int_0^T \int_0^t (\mathbf{q} \cdot \nabla \bar{U}^f_{\Delta t}(\tau), \phi_f(t))_{\Omega_f} d\tau dt - \int_0^T \int_0^t (\bar{f}_f(\tau), \phi_f(t))_{\Omega_f} d\tau dt \\
&- \int_0^T \int_0^t (\bar{f}_p(\tau), \phi_p(t))_{\Omega_p} d\tau dt - \int_0^T (u_{I,f}, \phi_f(t))_{\Omega_f} dt - \int_0^T (u_{I,p}, \phi_p(t))_{\Omega_p} dt \\
&= \sum_{k=1}^N \int_{t_{k-1}}^{t_k} \int_t^{t_k} (\bar{f}_f(\tau), \phi_f(t))_{\Omega_f} d\tau dt + \sum_{k=1}^N \int_{t_{k-1}}^{t_k} \int_t^{t_k} (\bar{f}_p(\tau), \phi_p(t))_{\Omega_p} d\tau dt \\
&- \sum_{k=1}^N \int_{t_{k-1}}^{t_k} \int_t^{t_k} (\nabla \bar{U}^f_{\Delta t}(\tau), \nabla \phi_f(t))_{\Omega_f} d\tau dt - \sum_{k=1}^N \int_{t_{k-1}}^{t_k} \int_t^{t_k} (\nabla \bar{U}^p_{\Delta t}(\tau), \nabla \phi_p(t))_{\Omega_p} d\tau dt \\
&- \sum_{k=1}^N \int_{t_{k-1}}^{t_k} \int_t^{t_k} (\mathbf{q} \cdot \nabla \bar{U}^f_{\Delta t}(\tau), \phi_f(t))_{\Omega_f} d\tau dt. \qquad (17)
\end{aligned}$$

By (16), for $\Delta t \searrow 0$ one has

$$\int_0^T (\bar{U}^i_{\Delta t}(t), \phi_i(t))_{\Omega_i} dt \to \int_0^T (U_i(t), \phi_i(t))_{\Omega_i} dt, \qquad (18)$$

$$\int_0^T \int_0^t (\nabla \bar{U}^i_{\Delta t}(\tau), \nabla \phi_i(t))_{\Omega_i} d\tau dt \to \int_0^T \int_0^t (\nabla U_i(\tau), \nabla \phi_i(t))_{\Omega_i} d\tau dt, \qquad (19)$$

$$\int_0^T \int_0^t (\mathbf{q} \cdot \nabla \bar{U}^f_{\Delta t}(\tau), \phi_f(t))_{\Omega_f} d\tau dt \to \int_0^T \int_0^t (\mathbf{q} \cdot \nabla U_f(\tau), \phi_f(t))_{\Omega_f} d\tau dt. \qquad (20)$$

Furthermore, since $f_i \in C(0,T;L^2(\Omega_i))$ we also have

$$\int_0^T \int_0^t (\bar{f}_i(\tau), \phi_i(t))_{\Omega_i} d\tau dt \to \int_0^T \int_0^t (f_i(\tau), \phi_i(t))_{\Omega_i} d\tau dt. \qquad (21)$$

We denote the terms on the right hand side of (17) by $T_1, ..., T_5$. Since $f_f \in C(0,T;L^2(\Omega_f))$, for T_1 one has

$$|T_1| \leq (\Delta t)^2 \sum_{k=1}^N ||f_f(t_k)||^2_{\Omega_f} + \frac{\Delta t}{4} ||\phi_f||^2_{\Omega_f} \leq C \Delta t,$$

with C independent of Δt. Therefore T_1 is vanishing as $\Delta t \searrow 0$.

For T_3 we use the priori estimate (12) to obtain

$$\begin{aligned}
|T_f| &\leq \sum_{k=1}^{N} \int_{t_{k-1}}^{t_k} \int_{t}^{t_k} \left|(\nabla \bar{U}^f_{\Delta t}(\tau), \nabla \phi_f(t))_{\Omega_f}\right| d\tau dt \\
&\leq \Delta t \sum_{k=1}^{N} \int_{t_{k-1}}^{t_k} \left|\left|\nabla u_f^k\right|\right|_{\Omega_f} ||\nabla \phi_f(t)||_{\Omega_i} \, dt \\
&\leq \Delta t \sum_{k=1}^{N} \int_{t_{k-1}}^{t_k} \left|\left|\nabla u_f^k\right|\right|^2_{\Omega_f} dt + \frac{\Delta t}{4} \sum_{k=1}^{N} ||\nabla \phi_f(t)||^2_{\Omega_f} \, dt \\
&\leq (\Delta t)^2 \sum_{k=1}^{N} \left|\left|\nabla u_f^k\right|\right|^2_{\Omega_f} + \frac{\Delta t}{4} \int_0^T ||\nabla \phi_f(t)||^2_{\Omega_f} \, dt \leq C \Delta t,
\end{aligned}$$

with C independent of Δt. This shows that T_3 vanishes as well as $\Delta t \searrow 0$.

The proofs for T_2, T_4 and T_5 are similar and we omit them here. This shows that for all $(\phi_f, \phi_p) \in L^2(0,T;V_f) \times L^2(0,T;V_p)$ s.t. $\phi_f = \phi_p$ on Γ, we have

$$\begin{aligned}
&\int_0^T (U_f(t), \phi_f(t))_{\Omega_f} dt + \int_0^T (U_p(t), \phi_p(t))_{\Omega_p} dt + \int_0^T \int_0^t (\nabla U_f(\tau), \nabla \phi_f(t))_{\Omega_f} d\tau dt \\
&+ \int_0^T \int_0^t (\nabla U_p(\tau), \nabla \phi_p(t))_{\Omega_p} d\tau dt + \int_0^T \int_0^t (\mathbf{q} \cdot \nabla U(\tau), \phi_f(t))_{\Omega_f} d\tau dt \\
&= \int_0^T \int_0^t (f_f(\tau), \phi_f(t))_{\Omega_f} d\tau dt + \int_0^T \int_0^t (f_p(\tau), \phi_p(t))_{\Omega_p} d\tau dt \qquad (22) \\
&+ \int_0^T (u_{I,f}, \phi_f(t))_{\Omega_f} dt + \int_0^T (u_{I,p}, \phi_p(t))_{\Omega_p} dt.
\end{aligned}$$

Next, let $\psi_i \in W^{1,2}(0,T;V_i)$ $(i = f,p)$ s.t. $\psi_f = \psi_p$ on Γ and $\psi_f(T) = \psi_p(T) = 0$. We observe that

$$\begin{aligned}
&\int_0^T \int_0^t (f_f(\tau), \partial_t \psi_f(t))_{\Omega_f} d\tau dt \\
&= -\int_0^T \int_{\Omega_f} f_f(t,x) \psi_f(t,x) dx dt + \int_{\Omega_f} \Big[\int_0^t f_f(\tau,x) d\tau \; \psi_f(t,x) \Big]_{t=0}^{t=T} dx \\
&= -\int_0^T (f_f(t), \psi_f(t))_{\Omega_f} dt.
\end{aligned}$$

Analogously, one gets similar results for the integrals involving f_p, as well as

$$\begin{aligned}
&\int_0^T \int_0^t (\nabla U_i(\tau), \nabla \partial_t \psi_i(t))_{\Omega_i} d\tau dt = -\int_0^T (\nabla U_i(t), \nabla \psi_i(t))_{\Omega_i} dt \; (i = f,p) \\
&\int_0^T \int_0^t (\mathbf{q} \cdot \nabla U_f(\tau), \partial_t \psi_f(t))_{\Omega_f} d\tau dt = -\int_0^T (\mathbf{q} \cdot \nabla U_f(t), \psi_f(t))_{\Omega_f} dt.
\end{aligned}$$

With $\phi_i := \partial_t \psi_i$ as test functions in (22) gives

$$\begin{aligned}
&\int_0^T (U_f(t), \partial_t \psi_f(t))_{\Omega_f} dt + \int_0^T (U_p(t), \partial_t \psi_p(t))_{\Omega_p} dt - \int_0^T (\nabla U_f(t), \nabla \psi_f(t))_{\Omega_f} dt \\
&- \int_0^T (\nabla U_p(t), \nabla \psi_p(t))_{\Omega_p} dt - \int_0^T (\mathbf{q} \cdot \nabla U_f(t), \psi_f(t))_{\Omega_f} dt \\
&= - \int_0^T (f_f(t), \psi_f(t))_{\Omega_f} dt - \int_0^T (f_p(t), \psi_p(t))_{\Omega_p} dt \\
&- (u_{I,f}, \psi_f(0))_{\Omega_f} - (u_{I,p}, \psi_p(0))_{\Omega_p}.
\end{aligned}$$

Therefore, (9) holds true.

It only remains to show that $U_f = r(U_p)$ on Γ. In doing so, we estimate

$$\begin{aligned}
||U_f - r(U_p)||_{\Gamma^T} \leq &\left|\left|U_f - \bar{U}^f_{\Delta t}\right|\right|_{\Gamma^T} \\
&+ \left|\left|r(U_p) - r(\bar{U}^p_{\Delta t})\right|\right|_{\Gamma^T} + \left|\left|\bar{U}^f_{\Delta t} - r(\bar{U}^p_{\Delta t})\right|\right|_{\Gamma^T}. \qquad (23)
\end{aligned}$$

The third term on the right vanishes since, by definition, $\bar{U}^f_{\Delta t} = r(\bar{U}^p_{\Delta t})$ on Γ. For the second term, by the trace inequality one has

$$\begin{aligned}
\left|\left|r(U_p) - r(\bar{U}^p_{\Delta t})\right|\right|^2_{\Gamma^T} &\leq M^2 \int_0^T \left|\left|U_p(t) - \bar{U}^p_{\Delta t}(t)\right|\right|^2_{\Gamma} dt \\
&\leq C \left|\left|U_p - \bar{U}^p_{\Delta t}\right|\right|_{\Omega_p^T} \left(\left|\left|\nabla U_p - \nabla \bar{U}^p_{\Delta t}\right|\right|_{\Omega_p^T} + \left|\left|U_p - \bar{U}^p_{\Delta t}\right|\right|_{\Omega_p^T} \right), \qquad (24)
\end{aligned}$$

with C only depending on the geometry of Ω_p. As $\Delta t \searrow 0$, $\left|\left|U_p - \bar{U}^p_{\Delta t}\right|\right|_{\Omega_p^T} \to 0$ by the strong convergence in Lemma 5. The weak convergence (16) implies that $\left|\left|\nabla U_p - \nabla \bar{U}^p_{\Delta t}\right|\right|_{\Omega_p^T}$ is bounded uniformly, and by (24) the second term on the right in (23) vanishes. A similar argument can be applied to the first term on the right, showing that the traces of U_f and $r(U_p)$ are equal a.e. on Γ. This concludes the proof.

3.4 Positivity and L^∞ bounds

As stated in Assumption A_I, the initial conditions are positive and essentially bounded. Since the Dirichlet boundary conditions are homogeneous one expects that the solution is positive and essentially bounded as well. This is proved below. We start with the proof for the time discrete concentrations u_f^k and u_p^k, which immediately give similar results for u_f and u_p. The procedure is quite standard and makes use of the nonpositive, respectively nonnegative cuts, $[\cdot]_+$ and $[\cdot]_-$:

$$[u]_+ := \begin{cases} 0, & \text{if } u \leq 0, \\ u, & \text{if } u > 0, \end{cases} \qquad [u]_- := \begin{cases} u, & \text{if } u < 0, \\ 0, & \text{if } u \geq 0. \end{cases} \qquad (25)$$

We start with the lower bounds, which are proved in

Lemma 6 *For any $k \in \{0,\dots,N\}$, $u_f^k \geq 0$ and $u_p^k \geq$ a.e..*

Proof The proof is by mathematical induction. By Assumption A_I, the statement holds for $k = 0$. Next, assuming $u_f^{k-1} \geq 0$ and $u_p^{k-1} \geq 0$ a.e., the same is obtained for u_f^k and u_p^k when testing in (10) with $\phi_f := [u_f^k]_-$ and $\phi_p := [r(u_p^k)]_-$. We omit the detailed arguments here, as these are standard.

For the upper bounds, with M, M_f, M_I introduced in the assumptions, we let $M_u := \max\{M_I, r(M_I), M_f, MM_f\}$ and prove

Lemma 7 *For all $k \in \{0,\dots,N\}$ one has*

$$u_f^k \leq M_u(k\Delta t + 1) \quad \text{and} \quad u_p^k \leq r^{-1}\big(M_u(k\Delta t + 1)\big).$$

Proof Here we use again mathematical induction and follow ideas in [8]. The statement holds trivially for $k = 0$. Next, assume $u_f^k \leq M_u\big((k-1)\Delta t+1\big)$ and $u_p^k \leq r^{-1}\Big(M_u\big((k-1)\Delta t+1\big)\Big)$. Since $u_f^k = r(u_p^k)$ on Γ, $\phi_f := [u_f^k - M_u(k\Delta t + 1)]_+$ and $\phi_p := [r(u_p^k) - M_u(k\Delta t + 1)]_+$ can be used as test functions in (10), giving

$$\begin{aligned}
&\big(u_f^k - M_u(k\Delta t + 1), \big[u_f^k - M_u(k\Delta t + 1)\big]_+\big)_{\Omega_f} \\
&+ \big(u_p^k - r^{-1}(M_u(k\Delta t + 1)), \big[r(u_p^k) - M_u(k\Delta t + 1)\big]_+\big)_{\Omega_p} \\
&+ \Delta t\big(\nabla(u_f^k - M_u k(\Delta t + 1)), \nabla\big[u_f^k - M_u k(\Delta t + 1)\big]_+\big)_{\Omega_f} \\
&+ \Delta t\big(\nabla(u_p^k - M_u k(\Delta t + 1)), \nabla\big[r(u_p^k) - M_u k(\Delta t + 1)\big]_+\big)_{\Omega_p} \\
&+ \Delta t\big(\mathbf{q}\cdot\nabla(u_f^k - M_u(k\Delta t + 1)), \big[u_f^k - M_u(k\Delta t + 1)\big]_+\big)_{\Omega_f} \\
=\ &\big(u_f^{k-1} - M_u((k-1)\Delta t + 1), \big[u_f^k - M_u(k\Delta t + 1)\big]_+\big)_{\Omega_f} \\
&+ \big(u_p^{k-1} - r^{-1}(M_u((k-1)\Delta t + 1)), \big[u_p^k - M_u(k\Delta t + 1)\big]_+\big)_{\Omega_p} \\
&+ \big(\Delta t f_p - r^{-1}(M_u(k\Delta t + 1)) + r^{-1}(M_u((k-1)\Delta t + 1)), \big[u_p^k - M_u(k\Delta t + 1)\big]_+\big)_{\Omega_p} \\
&+ \Delta t\big(f_f - M_u, \big[u_f^k - M_u(k\Delta t + 1)\big]_+\big)_{\Omega_f}. \qquad (26)
\end{aligned}$$

The first three terms in (26) are positive, while for the fourth one uses the properties of r to obtain

$$\big(\nabla(u_p^k - M_u k(\Delta t+1)), \nabla[r(u_p^k) - M_u k(\Delta t+1)]_+\big)_{\Omega_p} \geq m\|\nabla[u_p^k - M_u k(\Delta t+1)]_+)\|^2_{\Omega_p}.$$

As in the proof of Lemma 1, the last term on the left vanishes.

Also, by the induction hypothesis, the first two terms on the right are nonpositive , and the same holds for the third by Assumption A_f and since $M_u \geq M_f$. Finally, for a.e. $x \in \Omega_p$, a $\xi_x \in \big(M_u((k-1)\Delta t + 1), M_u(k\Delta t + 1)\big)$ exists s.t.

$$\begin{aligned}
&\Delta t f_p - \big(r^{-1}(M_u(k\Delta t + 1)) - r^{-1}(M_u((k-1)\Delta t + 1))\big) \\
&= \Delta t f_p - (r^{-1})'(\xi_x) M_u \Delta t \leq \Delta t M_{f_p} - \frac{1}{M} M_u \Delta t \leq 0.
\end{aligned}$$

Therefore the last term is nonpositive as well, showing that $u_f^k \le M_u(k\Delta t+1)$ and $u_p^k \le r^{-1}\big(M_u(k\Delta t+1)\big)$ a.e..

Lemmata 6 and 7 provide similar bounds for the solution pair (u_f, u_p).

Lemma 8 *The solution pair in Definition 3 is essentially bounded. For a.e.* $t \in [0,T]$ *one has*

$$0 \le u_f(t) \le M_u(t+1) \qquad \text{almost everywhere in } \Omega_f, \tag{27}$$

$$0 \le u_p(t) \le \frac{M_u}{m}(t+1) \qquad \text{almost everywhere in } \Omega_p. \tag{28}$$

Proof The proof uses the convergence of the interpolations in (13) and (14). In view of the results above, these are nonnegative a.e.. Further, the upper bounds follow straightforwardly for the interpolations in the fracture subdomain, and by using Remark 1 for the interpolation in the porous block.

4 Formal upscaling

We use the formal asymptotic expansions for the variables and use the transverse averaging to obtain the upscaled equations. Specifically, we let the fracture thickness ε go to zero and reduce the fracture model to a boundary condition. We refer to [9,25] for a general procedure applied to convection dominated regimes, and to [19,30,31] for more specific applications related to precipitation-dissolution models, or to biofilm growth in porous media. However, these papers refer strictly to the fracture region and do not consider the coupling with a porous block. For simplicity, a Poiseuille flow is considered, but the procedure can be applied to more general situations straightforwardly:

$$\mathbf{q} = (q^\varepsilon(y), 0), \qquad \text{with } q^\varepsilon(y) = \frac{3}{2}Q\frac{y}{\varepsilon}\Big(2-\frac{y}{\varepsilon}\Big). \tag{29}$$

Here Q is the average of the fluid velocity in the longitudinal direction, $Q = \frac{1}{2\varepsilon}\int_0^{2\varepsilon} q_{if}^\varepsilon(y)dy$, with $Q>0$. By this choice, the given velocity field satisfied the Stokes equation, and its transversal average does not vanish as $\varepsilon \searrow 0$.

For the upscaling we use the transformation $z := y/\varepsilon$ to rescale the fracture domain to $\Omega_f = (0,1)\times(0,1)$. However, the porous block Ω_p remains unchanged. For consistency, we change the name of the transversal variable y into z there as well. In this context, the upper part of the boundary becomes $\Gamma_f^2 = (0,1)\times\{1\}$, and (6) transforms into

$$\begin{cases} \partial_t u_p^\varepsilon - \Delta u_p^\varepsilon = f_p, & \text{in } (0,T]\times\Omega_p,\\ \partial_t u_f^\varepsilon + q^\varepsilon \partial_x u_f^\varepsilon - (\partial_{xx} u_f^\varepsilon + \frac{1}{\varepsilon^2}\partial_{zz} u_f^\varepsilon) = f_f, & \text{in } (0,T]\times\Omega_f,\\ u_f^\varepsilon = r(u_p^\varepsilon), & \text{at } (0,T]\times\Gamma,\\ \partial_z u_p^\varepsilon = \frac{1}{\varepsilon}\partial_z u_f^\varepsilon, & \text{at } (0,T]\times\Gamma,\\ \partial_z u_f^\varepsilon = 0, & \text{at } (0,T]\times\Gamma_f^2. \end{cases} \tag{30}$$

Observe that the partial derivatives $\frac{\partial}{\partial y}$ become now $\frac{1}{\varepsilon}\frac{\partial}{\partial z}$, and that $q^\varepsilon = q^\varepsilon(z) = \frac{3}{2}Qz(2-z)$.

In the fracture domain we redefine $\tilde{u}_f^\varepsilon$ in terms of the new variable z, $\tilde{u}_f^\varepsilon(t,x,z) = u_f^\varepsilon(t,x,\varepsilon z)$. By an abuse of notation allowing to avoid an excess of symbols, we give up the $\tilde{}$. Further, we assume the following asymptotic expansions for the pair $(u_f^\varepsilon, u_p^\varepsilon)$:

$$u_f^\varepsilon(t,x,z) = u_0^f(t,x,z) + \varepsilon u_1^f(t,x,z) + \mathcal{O}(\varepsilon^2), \tag{31}$$

$$u_p^\varepsilon(t,x,z) = u_0^p(t,x,z) + \varepsilon u_1^p(t,x,y) + \mathcal{O}(\varepsilon^2). \tag{32}$$

Substituting the expansions (31) and (32) in (30) gives

$$\partial_t(u_0^p + \varepsilon u_1^p) - \Delta(u_0^p + \varepsilon u_1^p) = f_p + \mathcal{O}(\varepsilon^2), \quad \text{in } (0,T]\times\Omega_p, \tag{33}$$

$$\partial_t u_0^f + \frac{3}{2}Qz(2-z)\partial_x u_0^f - \partial_{xx}u_0^f - \frac{1}{\varepsilon^2}\partial_{zz}(u_0^f + \varepsilon u_1^f + \varepsilon^2 u_2^f) = f_f + \mathcal{O}(\varepsilon), \quad \text{in } (0,T]\times\Omega_f, \tag{34}$$

$$u_0^f + \varepsilon u_1^f = r(u_0^p) + \varepsilon r'(u_0^p)u_1^p + \mathcal{O}(\varepsilon^2), \quad \text{at } (0,T]\times\Gamma, \tag{35}$$

$$\partial_z(u_0^p + \varepsilon u_1^p) = \frac{1}{\varepsilon}\partial_z(u_0^f + \varepsilon u_1^f + \varepsilon^2 u_2^f) + \mathcal{O}(\varepsilon), \quad \text{at } (0,T]\times\Gamma, \tag{36}$$

$$\partial_z(u_0^f + \varepsilon u_1^f + \varepsilon^2 u_2^f) = \mathcal{O}(\varepsilon^3), \quad \text{at } (0,T]\times\Gamma_f^2. \tag{37}$$

The ε^{-2} term in (34), and the lowes order terms in (36) and (37) imply

$$\partial_{zz}u_0^f = 0, \quad \text{in } \Omega_f, \qquad \text{and} \qquad \partial_z u_0^f = 0, \quad \text{at } \Gamma_f^2 \cup \Gamma.$$

This gives

$$u_0^f(x,z,t) = u_0^f(x,t).$$

In a similar fashion one gets

$$u_1^f(x,z,t) = u_1^f(x,t).$$

Hence, from equation (36), we obtain

$$\partial_z u_0^p = 0, \qquad \text{at } (0,T]\times\Gamma. \tag{38}$$

The ε^0 term of (35) gives

$$u_0^f = r(u_0^p), \qquad \text{at } (0,T]\times\Gamma. \tag{39}$$

Furthermore, the ε^0 term of (33) implies

$$\partial_t u_0^p - \Delta u_0^p = f_p, \qquad \text{in } (0,T]\times\Omega_p. \tag{40}$$

From the above, one obtains the effective model

$$(P_{\mathrm{UP}_0}) \begin{cases} \partial_t u_0^p - \Delta u_0^p = f_p, & \text{in } (0,T]\times\Omega_p, \\ \partial_z u_0^p = 0, & \text{at } (0,T]\times\Gamma, \\ u_0^f = r(u_0^p), & \text{at } (0,T]\times\Gamma. \end{cases} \tag{41}$$

The model above is completed by the initial conditions and the (homogeneous) Dirichlet boundary conditions as stated in Section 2. Note that u_0^p can be solved independently of u_0^f. The last boundary condition in 41 provides the effective concentration in the fracture, u_0^f.

4.1 Higher order approximation

The procedure above can be continued to find effective equations having better approximation properties than (41). To this end, we consider the ε^0 term of equation (34),

$$\partial_t u_0^f - Q\frac{3}{2}z(z-2)\partial_x u_0^f - \partial_{xx} u_0^f - \partial_{zz} u_2^f = f_f \qquad \text{in } \Omega_f. \tag{42}$$

Integrating (42) from $z=0$ to $z=1$, since u_0^f does not depend on z and using (37) one gets

$$\partial_t u_0^f + Q\partial_x u_0^f - \partial_{xx} u_0^f - \bar{f}_f = \partial_z u_2^f\big|_{z=0}^{z=1},$$

for $(t,x) \in (0,T]\times(0,1)$, where $\bar{f}_f := \int_{-1}^{0} f_f dz$. By (36) and (37), this becomes

$$-\partial_z u_1^p\big|_{z=0} = \partial_t u_0^f + Q\partial_x u_0^f - \partial_{xx} u_0^f - \bar{f}_f. \tag{43}$$

The ε^1 term of (35) gives

$$u_1^f = r'(u_0^p)u_1^p, \qquad \text{at } (0,T]\times\Gamma, \tag{44}$$

and the ε^1 term of (33) implies

$$\partial_t u_1^p - \Delta u_1^p = 0, \qquad \text{in } (0,T]\times\Omega_p. \tag{45}$$

Defining the effective quantities

$$u_e^p := u_0^p + \varepsilon u_1^p, \quad \text{and} \quad u_e^f := u_0^f + \varepsilon u_1^f, \tag{46}$$

adding (38) to (43), (39) to (44), and (40) to (45) gives

$$\partial_t u_e^p - \Delta u_e^p = f_p, \qquad \text{in } (0,T]\times\Omega_p, \tag{47}$$

$$u_e^f = r(u_0^p) + \varepsilon r'(u_0^p)u_1^p, \qquad \text{at } (0,T]\times\Gamma, \tag{48}$$

$$-\partial_z u_e^p = \varepsilon\Big(\partial_t u_0^f + Q\partial_x u_0^f - \partial_{xx} u_0 - \bar{f}_f\Big), \qquad \text{at } (0,T]\times\Gamma. \tag{49}$$

Up to ε^2 terms, (47)-(49) becomes

$$(P_{\mathrm{Up}_1}) \begin{cases} \partial_t u_e^p = \Delta u_e^p + f_p, & \text{in } (0,T]\times\Omega_p, \\ -\partial_z u_e^p = \varepsilon(\partial_t u_e^f + Q\partial_x u_e^f - \partial_{xx} u_e^f - \bar{f}_f), & \text{at } (0,T]\times\Gamma, \\ u_e^f = r(u_e^p), & \text{at } (0,T]\times\Gamma. \end{cases} \tag{50}$$

As before, initial and boundary conditions complete the model. Furthermore, substituting the third equation in the second one leads to a (nonlinear) model only in terms of u_e^p, and again can be solved independently. Then u_e^f can be determined from the third equation.

4.2 Formal upscaling of drift dominated model

As for the original model, we now determine upscaled (effective) equations for the model with dominating drift, where $Pe = \mathcal{O}(\varepsilon^{-1})$. Our approach is inspired from similar exercises carried out for precipitation-dissolution type models in [19,25], but uses the drift model discussed e.g. in [1,2,3], and assumes that the velocity is now very high, i.e. of order ε^{-1}. The system of equations is given by

$$\begin{cases} \partial_t u_p^\varepsilon - \Delta u_p^\varepsilon = f_p^\varepsilon, & \text{in } (0,T]\times\Omega_p, \\ \partial_t u_f^\varepsilon + \frac{1}{\varepsilon}\mathbf{q}^\varepsilon\cdot\nabla u_f^\varepsilon - \Delta u_f^\varepsilon = f_f^\varepsilon, & \text{in } (0,T]\times\Omega_f^\varepsilon, \\ u_f^\varepsilon = r(u_p^\varepsilon), & \text{at } (0,T]\times\Gamma, \\ \partial_{\boldsymbol{\nu}} u_p^\varepsilon = \partial_{\boldsymbol{\nu}} u_f^\varepsilon, & \text{at } (0,T]\times\Gamma. \end{cases} \tag{51}$$

We proceed agian by rescaling the fractured domain. Using the asymptotic expansions (31) - (32), (51) becomes

$$\partial_t(u_0^p+\varepsilon u_1^p) - \Delta(u_0^p+\varepsilon u_1^p) = f_p + \mathcal{O}(\varepsilon^2), \quad \text{in } (0,T]\times\Omega_p, \tag{52}$$

$$\partial_t u_0^f + \frac{3}{2\varepsilon}Qz(2-z)\partial_x u_0^f - \partial_{xx}u_0^f - \frac{1}{\varepsilon^2}\partial_{zz}(u_0^f+\varepsilon u_1^f+\varepsilon^2 u_2^f) = f_f + \mathcal{O}(\varepsilon), \quad \text{in } (0,T]\times\Omega_f, \tag{53}$$

$$u_0^f + \varepsilon u_1^f = r(u_0^p) + \varepsilon r'(u_0^p)u_1^p + \mathcal{O}(\varepsilon^2), \quad \text{at } (0,T]\times\Gamma, \tag{54}$$

$$\partial_z(u_0^p+\varepsilon u_1^p) = \frac{1}{\varepsilon}\partial_z(u_0^f+\varepsilon u_1^f+\varepsilon^2 u_2^f) + \mathcal{O}(\varepsilon), \quad \text{at } (0,T]\times\Gamma, \tag{55}$$

$$\partial_z(u_0^f+\varepsilon u_1^f+\varepsilon^2 u_2^f) = \mathcal{O}(\varepsilon^3), \quad \text{at } (0,T]\times\Gamma_f^2. \tag{56}$$

As before, we obtain $u_0^f(x,z,t) = u_0^f(x,t)$. Further, the ε^{-1} terms in (53) give

$$-\frac{3}{2}Qz(z-2)\partial_x u_0^f - \partial_{zz}u_1^f = 0, \qquad \text{in } \Omega_f. \tag{57}$$

Integrating (57) from $z=0$ to $z=1$, using that u_0 is independent of z and the boundary condition (56) yields

$$-Q\partial_x u_0^f = \partial_z u_1^f\big|_{z=0}.$$

Using the ε^0 terms in (55), this gives

$$-\partial_z u_0^p = Q\partial_x u_0^f, \qquad \text{at } (0,T]\times\Gamma. \tag{58}$$

Furthermore, the ε^0 term from (54) implies

$$u_0^f = r(u_0^p), \qquad \text{on } \Gamma,$$

and the ε^0 term of (52) gives

$$\partial_t u_0^p - \Delta u_0^p = f_p, \qquad \text{in } \Omega_p.$$

Summarizing, the leading order terms solve the model

$$(P_{\mathrm{Dr}_0})\begin{cases}\partial_t u_0^p - \Delta u_0^p = f_p, & \text{in } (0,T]\times\Omega_p,\\ -\partial_z u_0^p = Q\partial_x u_0^f, & \text{at } (0,T]\times\Gamma,\\ u_0^f = r(u_0^p), & \text{at } (0,T]\times\Gamma.\end{cases} \tag{59}$$

Boundary and initial conditions are needed to complete the model, which, as before can be reduced to the a (nonlinear) model in u_0^p.

Further, a more accurate model, is obtained when including higher order terms. The ε^0 term in (53) is

$$\partial_t u_0^f + \frac{3}{2}Qz(2-z)\partial_x u_1^f - \partial_{xx}u_0^f - \partial_{zz}u_2^f = f_f. \tag{60}$$

Integrating (60) from $z=0$ to $z=1$ gives for $(t,x)\in(0,T]\times(0,1)$

$$\partial_t u_0^f - \int_0^1 \frac{3}{2}Qz(z-2)\partial_x u_1^f dz - \partial_{xx}u_0^f - \bar{f}_f = -\partial_z u_2^f\big|_{z=0}^{z=1},$$

where $\bar{f}_f = \int_0^1 f_f dz$. Hence, by (55) and (56), we have

$$-\partial_z u_1^p\big|_{z=0} = \partial_t u_0^f - \int_0^1 \frac{3}{2}Qz(z-2)\partial_x u_1^f dz - \partial_{xx}u_0^f - \bar{f}_f. \tag{61}$$

With the effective quantities

$$u_e^p := u_0^p + \varepsilon u_1^p \text{ and } u_e^f := u_0^f + \varepsilon\bar{u}_1^f, \text{ where } \bar{u}_1^f := \int_0^1 u_1^f dz,$$

adding (58) and (61) gives

$$-\partial_z u_e^p = Q\partial_x u_0^f + \varepsilon\Big(\partial_t u_0^f - \int_0^1 \frac{3}{2}Qz(z-2)\partial_x u_1^f dz - \partial_{xx}u_0^f - \bar{f}_f\Big). \tag{62}$$

By (57), in $(0,T]\times\Omega_f$ one has

$$\partial_z u_1^f = \frac{3}{2}Q\partial_x u_0^f\big(\frac{z^2-z^3}{3}\big) + c_1(x,t).$$

Since $\partial_z u_1 = 0$ at Γ_f^2, we get $c_1(x,t) = -Q\partial_x u_0^f$. This gives

$$u_1^f = -\frac{3}{2}Q\big(\frac{z^4}{12} - \frac{z^3}{3}\big)\partial_x u_0^f - Qz\partial_x u_0^f + c_2(x,t).$$

Integrating the above from $z=0$ to $z=1$, and after some elementary calculations, one has $c_2(x,t) = \bar{u}_1^f + \frac{2}{5}Q\partial_x u_0^f$, hence

$$u_1^f(x,z,t) = -\frac{3}{2}Q\big(\frac{z^4}{12} - \frac{z^3}{3}\big)\partial_x u_0^f - Qz\partial_x u_0^f + \bar{u}_1^f + \frac{2}{5}Q\partial_x u_0^f. \tag{63}$$

This can be used to compute

$$\int_0^1 \frac{3}{2}Qz(z-2)\partial_x u_1^f dz = \frac{3}{35}Q^2\partial_{xx}u_0^f - Q\partial_x \bar{u}_1^f.$$

Inserting this in (62) gives for $(t,x) \in (0,T] \times (0,1)$

$$\begin{aligned}-\partial_z u_e^p &= Q\partial_x u_0^f + \varepsilon\Big(\partial_t u_0^f - \frac{3}{35}Q^2\partial_{xx}u_0^f + Q\partial_x \bar{u}_1^f - \partial_{xx}u_0^f - \bar{f}_f\Big)\\ &= Q\partial_x u_e^f + \varepsilon\Big(\partial_t u_0^f - \big(1+\frac{3}{35}Q^2\big)\partial_{xx}u_0^f - \partial_{xx}u_0^f - \bar{f}_f\Big).\end{aligned}$$

Up to an $O(\varepsilon^2)$ error, this rewrites

$$-\partial_z u_e^p = Q\partial_x u_e^f + \varepsilon\Big(\partial_t u_e^f - \big(1+\frac{3}{35}Q^2\big)\partial_{xx}u_e^f - \bar{f}_f\Big).$$

Similarly, the nonlinear transmission condition becomes

$$r(u_p^\varepsilon|_{z=0}) = r(u_e^p|_{z=0}) + O(\varepsilon^2).$$

Furthermore, using the expression for u_1^f obtained in (63), we have

$$\begin{aligned}u_f^\varepsilon|_{z=0} &= u_e^f + \varepsilon(u_1^f|_{z=0} - \bar{u}_1^f) + O(\varepsilon^2)\\ &= u_e^f + \varepsilon\frac{2Q}{5}\partial_x u_0^f + O(\varepsilon^2) = u_e^f + \varepsilon\frac{2Q}{5}\partial_x u_e^f + O(\varepsilon^2).\end{aligned}$$

Adding the ε^0 and ε^1 terms of (52), gives

$$\partial_t u_e^p - \Delta u_e^p = f_p, \qquad \text{in } \Omega_p.$$

Summarizing, we have the following set of effective equations

$$(P_{\mathrm{Dr}_1})\begin{cases} \partial_t u_e^p = \Delta u_e^p + f_p, & \text{in } (0,T]\times\Omega_p,\\ -\partial_z u_e^p = Q\partial_x u_e^f & \\ \qquad + \varepsilon\Big(\partial_t u_e^f - \big(1+\frac{3Q^2}{35}\big)\partial_{xx}u_e^f - \bar{f}_f\Big), & \text{at } (0,T]\times\Gamma,\\ r(u_e^p) = u_e^f + \frac{2Q}{5}\partial_x u_e^f, & \text{at } (0,T]\times\Gamma. \end{cases} \tag{64}$$

In this particular situation, the third equation gives

$$u_e^f = e^{-\frac{5}{2Q}x}\int_0^x \frac{5}{2Q}e^{\frac{5}{2Q}\xi} r(u_e^p)d\xi, \tag{65}$$

allowing again to decouple the problem for u_e^p.

5 Rigorous upscaling for moderate Peclét ($Pe = O(1)$)

In this Section we give a rigorous convergence proof for the upscaled model obtained in Section 4, when diffusion and transport are in balance. We follow ideas from [11], pp.200-208 (a detailed presentation can be found in [4], Chapters 4 and 9; see also [18] for an extension of the results to periodic media, and [12] for a similar dimensionality reduction approach). As in the formal upscaling, to simplify the exposition we assume the parabolic velocity profile in (29). For the proofs we derive ε-independent a priori estimates, and use compactness arguments to pass to the limit. Note that most of these a priori estimates immediately follow from the ones already obtained when proving existence.

5.1 Weak formulation

As in Section 4, the fractured part is rescaled verticallly by $z = y/\varepsilon$. Then $0 < z < 1$ and the domain Ω_f^ε transforms to $\Omega_f = (0,1) \times (0,1)$. Furthermore, $q^\varepsilon(z) = q(z) := -\frac{3}{2}Qz(z-2)$. We define,

$$\tilde{u}_f^\varepsilon(t,x,z) := u_f^\varepsilon(t,x,z\varepsilon),\ \tilde{f}_f(t,x,z) := f_f(t,x,z\varepsilon),\ \tilde{u}_{I,f}(x,z) := u_{I,f}(x,z\varepsilon).$$

We have $\tilde{u}_f^\varepsilon \in L^2(0,T;V_f)$, $\tilde{u}_f^\varepsilon = r(u_p^\varepsilon)$ on Γ and (3) becomes

$$\begin{aligned}
&-(u_p^\varepsilon, \partial_t\phi_p)_{\Omega_p^T} - \varepsilon(\tilde{u}_f^\varepsilon, \partial_t\phi_f)_{\Omega_f^T} + D_p(\nabla u_p^\varepsilon, \nabla\phi_p)_{\Omega_p^T} + \varepsilon D_f(\partial_x\tilde{u}_f^\varepsilon, \partial_x\phi_f)_{\Omega_f^T} \\
&+ \frac{D_f}{\varepsilon}(\partial_z\tilde{u}_f^\varepsilon, \partial_z\phi_f)_{\Omega_f^T} + \varepsilon(q\partial_x\tilde{u}_f^\varepsilon, \phi_f)_{\Omega_f^T} \\
&= (f_p^\varepsilon, \phi_p)_{\Omega_p^T} + \varepsilon(\tilde{f}_f^\varepsilon, \phi_f)_{\Omega_f^T} + (u_{I,p}, \phi_p(0))_{\Omega_p} + \varepsilon(\tilde{u}_{I,f}, \phi_f(0))_{\Omega_f}
\end{aligned} \tag{66}$$

for all $(\phi_f, \phi_p) \in W^{1,2}(0,T,V_f) \times W^{1,2}(0,T,V_p)$ such that $\phi_p = \phi_f$ on Γ, and $\phi_f(T) = \phi_p(T) = 0$.

In the fracture, we define the (vertical) average

$$U_f^\varepsilon(t,x) := \int_0^1 \tilde{u}_f^\varepsilon(t,x,z)dz.$$

Furthermore, we let $\Omega_{AV} := (0,1)$. Since $\tilde{u}_f^\varepsilon \in L^2(0,T;V_f^\varepsilon)$, $U_f^\varepsilon \in L^2(0,T;W_0^{1,2}(\Omega_{AV}))$. For consistency of notation, we let $U_p(t,x,z) := u_p(t,x,z)$. We also define $\bar{f}_f(t,x) := \int_0^1 \tilde{f}_f(t,x,z)dz$ and $\bar{u}_{I,f}(x) := \int_0^1 \tilde{u}_{I,f}(x,z)dz$.

Below we show that as $\varepsilon \searrow 0$, the pair $(U_p^\varepsilon, U_f^\varepsilon)$ converges towards (U_p, U_f), the weak solution of the upscaled Problem P_{Up_0} in (41). This is defined below

Definition 6 *A pair $(U_f, U_p) \in L^2(0,T;L^2(\Omega_{AV})) \times L^2(0,T;V_p)$ is a weak solution to Problem P_{Up_0} if for the trace of U_p on Γ one has $U_f = r(U_p)$, and*

$$-(U_p, \partial_t\phi_p)_{\Omega_p^T} + (\nabla U_p, \nabla\phi_p)_{\Omega_p^T} = (f_p, \phi_p)_{\Omega_p^T} + (u_{I,p}, \phi_p(0))_{\Omega_p},$$

for all $\phi_p \in W^{1,2}(0,T;V_p)$ such that $\phi_p(T) = 0$.

In the convergence proof the transversal average of the fracture model will be used. For estimating this we test in (66) with z-independent functions in the fracture, that is, $\phi_f(t,x,z) = \phi_f(t,x)$. This gives

$$\begin{aligned}
&-\varepsilon(U_f^\varepsilon, \partial_t\phi_f)_{(\Omega_{AV})^T} - (U_p^\varepsilon, \partial_t\phi_p)_{\Omega_p^T} + (\nabla U_p^\varepsilon, \nabla\phi_p)_{\Omega_p^T} \\
&+\varepsilon(\partial_x U_f^\varepsilon, \partial_x\phi_f)_{\Omega_{AV}^T} + \varepsilon Q(\partial_x U_f^\varepsilon, \phi_f)_{\Omega_{AV}^T} \\
=&\,\varepsilon(\bar{f}_f, \phi_f)_{\Omega_{AV}^T} + (f_p, \phi_p)_{\Omega_p^T} + \varepsilon(\int_0^1 (Q-q)\partial_x u_f^\varepsilon, \phi_f)_{\Omega_{AV}^T} \\
&+\varepsilon(\bar{u}_{I,f}, \phi_f(0))_{\Omega_{AV}} + (u_{I,p}, \phi_p(0))_{\Omega_{AV}},
\end{aligned} \tag{67}$$

for all $(\phi_f, \phi_p) \in L^2(0,T,W_0^{1,2}(\Omega_{AV})) \times L^2(0,T,V_p)$ such that $\phi_p = \phi_f$ on Γ, and $\phi_f(T) = \phi_p(T) = 0$. We now pass to the limit $\varepsilon \searrow 0$ in (67). To do so, we adapt the proofs in Section 3.2 to obtain the a priori estimates

Lemma 9 *There exists $C > 0$ independent of ε such that*

$$\left|\left|u_p^\varepsilon\right|\right|^2_{L^2(0,T;V_p)} + \varepsilon \left|\left|\partial_x \tilde{u}_f^\varepsilon\right|\right|^2_{\Omega_f^T} + \frac{1}{\varepsilon}\left|\left|\partial_z \tilde{u}_f^\varepsilon\right|\right|^2_{\Omega_f^T} \leq C.$$

Similar estimates can be obtained for U_p^ε and U_f^ε:

Lemma 10 *There exists a constant $C > 0$ not depending on ε such that*

$$\left|\left|U_p^\varepsilon\right|\right|^2_{L^2(0,T;V_p)} + \left|\left|U_f^\varepsilon\right|\right|^2_{\Omega_{AV}^T} + \varepsilon\left|\left|\partial_x U_f^\varepsilon\right|\right|^2_{\Omega_{AV}^T} \leq C.$$

Moreover, the essential bounds in Lemma 8 remain valid for U_p^ε and U_f^ε. For all $t \in (0,T]$,

$$0 \leq U_f^\varepsilon(t) \leq M_u(t+1) \text{ almost everywhere in } \Omega_{AV}, \tag{68}$$

$$0 \leq U_p^\varepsilon(t) \leq \frac{M_u}{m}(t+1) \text{ almost everywhere in } \Omega_p. \tag{69}$$

This implies the weak convergence

$$U_p^\varepsilon \rightharpoonup U_p, \quad \text{weakly in } L^2(0,T;V_p), \tag{70}$$

$$U_f^\varepsilon \rightharpoonup U_f, \quad \text{weakly in } L^2(0,T;L^2(\Omega_{AV})). \tag{71}$$

Next, as for Lemma 5 one obtains the strong convergence of U_p^ε to U_p in $L^2(0,T;L^2(\Omega_p))$, providing the strong convergence for the traces on Γ.

Lemma 11 *Along a sequence $\varepsilon \searrow 0$, one has*

$$U_p^\varepsilon \to U_p \qquad \text{strongly in } L^2(0,T;L^2(\Omega_p)).$$

Finally, combining Lemma 9 and Proposition 4.3 in [11] gives

Lemma 12 *There exists a $C > 0$ not depending on ε s.t. for any $z_0 \in [0,1]$ one has*

$$\left|\left|\tilde{u}_f^\varepsilon(\cdot,\cdot,z_0) - U_f^\varepsilon\right|\right|^2_{\Omega_{AV}^T} \leq \varepsilon C.$$

Using this, one can follow the steps in the proof of Lemma 4.5 in [11] to obtain

Lemma 13 *A constant $C > 0$ not depending on ε exists such that for all $\phi_f \in L^2(0,T;W_0^{1,2}(\Omega_{AV}))$*

$$\left|\Big(\int_0^1 (Q-q)dz\partial_x\tilde{u}_f^\varepsilon,\phi_f\Big)_{\Omega_{AV}^T}\right| \leq Q\sqrt{\frac{53C}{40}}\,||\partial_x\phi_f||_{L^2(\Omega_{AV}^T)}.$$

We now have sufficient estimates to let $\varepsilon \searrow 0$, and show that the limiting pair (U_p, U_f) is a weak solution introduced in Definition 6. The result is contained in the following theorem.

Theorem 7 *The pair (U_p, U_f) is a weak solution introduced in Definition 6.*

Proof For arbitrary test functions, we denote the terms of (67) by $I_1, ..., I_{10}$ and analyze their limit as $\varepsilon \searrow 0$. The weak convergence in (70) gives

$$I_2 \to -(U_p, \partial_t\phi_p)_{\Omega_p^T},$$
$$I_3 \to (\nabla U_p, \nabla\phi_p)_{\Omega_p^T}.$$

Further, by Lemma 10 one has

$$|I_1| \leq \varepsilon|(U_f^\varepsilon, \partial_t\phi_f)_{\Omega_{AV}^T}| \leq \varepsilon\left|\left|U_f^\varepsilon\right|\right|_{\Omega_{AV}^T}||\partial_t\phi_f||_{\Omega_{AV}^T} \leq C\varepsilon\,||\partial_t\phi_f||_{\Omega_{AV}^T} \to 0.$$

The argument can be repeated for I_4, I_5, I_6 and I_9 to conclude that all have 0 limit as well. Moreover, by Lemma 13, the same holds for I_8.

The terms I_7 and I_{10} do not change in the limit, since they do not depend on ε. Hence, for all $\phi_p \in W^{1,2}(0,T;V_p)$ such that $\phi_p(T) = 0$, U_p satisfies

$$-(U_p, \partial_t\phi_p)_{\Omega_p^T} + (\nabla U_p, \nabla\phi_p)_{\Omega_p^T} = (f_p, \phi_p)_{\Omega_p^T} + (u_{I,p}, \phi_p(0))_{\Omega_p}.$$

It remains to show that $r(U_p) = U_f$ on Γ. To this end, for arbitrary $\phi \in L^2(0,T;L^2(\Gamma))$ we use the triangle inequality to estimate

$$\begin{aligned}|(r(U_p) - U_f, \phi)_{\Gamma^T}| \leq\ & |(r(U_p^\varepsilon) - r(U_p), \phi)_{\Gamma^T}| + |(U_f^\varepsilon - U_f, \phi)_{\Gamma^T}| \\ & + |(r(u_p^\varepsilon) - \tilde{u}_f^\varepsilon, \phi)_{\Gamma^T}| + |(U_f^\varepsilon - \tilde{u}_f^\varepsilon, \phi)_{\Gamma^T}|.\end{aligned}$$

We denote the terms on the right hand side by $\tilde{I}_1, ..., \tilde{I}_4$ and let $\varepsilon \searrow 0$. For $\tilde{I}_1$ we follow the steps concluding the proof of Theorem 5, namely use the trace inequality, (70) and the strong convergence in Lemma 11 to conclude that $\left|\left|r(U_p^\varepsilon) - r(U_p)\right|\right|_{\Gamma^T}$ vanishes, implying that $\tilde{I}_1 \to 0$. Next, $\tilde{I}_2$ goes to zero by the weak convergence (71). $\tilde{I}_3 = 0$ trivially, by the nonlinear transmission condition, and $\tilde{I}_4$ goes to zero by Lemma 12. Finally, since $\phi \in L^2(0,T;L^2(\Gamma))$ was chosen arbitrarily, we conclude that $U_f = r(U_p)$ on Γ, finishing the proof.

6 Discussion and outlook

We have derived upscaled equations for a time dependent reactive transport process in a fractured porous domain. The particularity lies in the nonlinear transmission conditions at the fracture interfaces. Both formal and rigorous upscaling procedures have been employed. The key role in this work is played by the existence results obtained in [14] for similar kind of elliptic problems. Related to this, efficient solution strategies for such kind of coupled problems need to be developed, including domain decomposition approaches as discussed in [5].

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