

Strong solvability up to clogging of an effective diffusion–precipitation model in an evolving porous medium

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In the first part of this article, we extend the formal upscaling of a diffusion–precipitation model through a two-scale asymptotic expansion in a level set framework to three dimensions. We obtain upscaled partial differential equations, more precisely, a non-linear diffusion equation with effective coefficients coupled to a level set equation. As a first step, we consider a parametrization of the underlying pore geometry by a single parameter, e.g. by a generalized “radius” or the porosity. Then, the level set equation transforms to an ordinary differential equation for the parameter. For such an idealized setting, the degeneration of the diffusion tensor with respect to porosity is illustrated with numerical simulations. The second part and main objective of this article is the analytical investigation of the resulting coupled partial differential equation–ordinary differential equation model. In the case of non-degenerating coefficients, local-in-time existence of at least one strong solution is shown by applying Schauder’s fixed point theorem. Additionally, non-negativity, uniqueness, and global existence or existence up to possible closure of some pores, i.e. up to the limit of degenerating coefficients, is guaranteed.

Key words: periodic homogenization; evolving microstructure; effective constitutive equations; finite element methods; strong solutions

1 Introduction

Diffusive transport in porous media is a thoroughly, investigated multi-scale problem, which has been studied in numerous publications. Traditionally, a porous medium is characterized by a rigid porous matrix. However, recently, the integration of an evolving porous matrix caused by, e.g. heterogeneous reactions has attracted increased interest. Consequently, new demands are being placed on multi-scale modeling, analysis, and numerics of such problems.

In the field of upscaling, the issue of deformable porous media has been treated in the following alternative approaches: On the one hand, mechanical aspects have been integrated to flow and transport models to account for small elastic deformations [14–16]. On the other hand, an extension of the homogenization technique including transformations to fixed domains has been introduced in [19] and applied in [13, 18, 20]. This is, however, restricted to a relatively smooth evolution of the porous matrix without topological change. In comparison, an approach capable of more flexible variations in geometry is introduced in [35]. More precisely, an extension of formal two-scale asymptotic expansion to a level set framework to capture the evolving solid–liquid interface was introduced for two space-dimensional applications. This formal method was recently applied to locally periodic media, biofilm growth, colloid dynamics, and drug delivery systems [24–26, 37, 38]. Finally, phase-field models that are based on a free energy functional are an alternative tackling the deformations of the porous medium or phase transitions. Homogenization techniques are applied to such models in [8, 27–30].

In the context of homogenization in non-rigid porous media, only a small number of analytical results is present in the literature: In [17, 37], upscaling of an advection–diffusion(–reaction) system in a locally periodic medium, including low and high diffusivities, was considered. Moreover, existence analysis was undertaken and an error estimate was obtained for the resulting upscaled system, which includes space-dependent but not time-dependent coefficients. Based on [34], in [36], the authors analysed dissolution and precipitation in one spatial dimension. In particular, existence and uniqueness were shown by transforming the model to a fixed domain. Likewise, in [5], root growth was considered and analysed further by a rigorous homogenization technique. Thereby, the evolution of root tips with a simple root geometry was modelled by an ordinary differential equation (ODE). The existence of weak solutions was shown for the microscopic model by applying a transformation to a fixed domain. An upscaled model describing the growth of biofilms in porous media was derived and its weak solvability was investigated in [31]. In [2], the existence of strong solutions for coupled system of an ODE and partial differential equations (PDEs) with non-constant coefficients and quadratic non-linearities, in the context of dopant diffusion in three dimensions, was shown. Thus far, however, little attention has been paid to the fact that upscaling flow and transport in evolving porous media may directly lead to systems of degenerate, PDEs, whose analytical investigation is hardly ever available. A comprehensive overview of degenerate parabolic equations was given, e.g. in [6]. Degenerate parabolic equations are often treated by applying Kirchhoff’s transformation [1]. In porous media applications, the problem of degeneration was already addressed with reference to this technique, among others, in the context of Richards’ equation, cf. [21, 22].

When modelling reactive transport including homogeneous and heterogeneous reactions, another difficulty arises: systems of non-linear ODEs and PDEs coupled to algebraic equations must be considered [12].

In this article, we consider diffusive transport in a saturated porous medium including precipitation at the porous matrix and revise the model’s upscaling by extending the theory of van Noorden [35] from two to three dimensions. In this locally periodic setting, we obtain a system of coupled, upscaled PDEs containing time- and space-dependent coefficient functions. As a first step, we consider a parametrization of the underlying

pore geometry by a single parameter that is, for example, related to a generalized “radius” or the porosity. Then, the level set equation transforms to an ODE for the parameter. Their regularity is analysed and the aforementioned degeneration of the diffusion tensor with respect to porosity is illustrated with numerical simulations. For such a simplified geometric setting, we first prove existence of at least one local-in-time solution of the resulting coupled PDE–ODE model by applying Schauder’s fixed point theorem. Moreover, positivity, uniqueness and global-in-time existence of strong solutions in case of non-degenerating coefficients, i.e. away from clogging, is shown. Beyond that result, uniqueness and existence is guaranteed up to the clogging of some pores, i.e. up to the limit of degenerating coefficients.

2 Mathematical model

In this section, we present a pore-scale model and an effective model describing diffusive transport in a porous medium and the species’ interaction with the porous matrix by heterogeneous reactions. In particular, the evolution of the porous matrix, i.e. of the solid–liquid interface is included into the model by means of a level set description. Moreover, the derivation of the effective model by asymptotic expansion in a level set framework in two and three dimensions is discussed. In this first part of the article, we strongly refer to [35] in which an extension to our model is considered, i.e. a moving fluid is included. However, all results presented therein are restricted to the two-dimensional case. We conversely focus on the three-dimensional setting and extend all analysis needed. In particular, we transfer [35, Lemma 3.1] and [35, Lemma 3.2] to three dimensions; these form the basis for the purpose of upscaling in a level set framework. Contrary to two dimensions, the introduction of a uniquely defined tangent vector orthogonal to the unit outer normal is not possible in three dimensions and as a consequence [35, Lemma 3.2] has to be reformulated in different terms.

2.1 Geometrical setting and pore-scale model

To set up the multi-scale framework, we first describe the underlying geometrical setting: We consider a bounded and connected domain $\Omega_0 \subset \mathbb{R}^n$, $n = 2, 3$, with exterior boundary $\partial\Omega_0$ and with an associated periodic microstructure. The microstructure is defined by unit cells $Y = [-\frac{1}{2}, +\frac{1}{2}]^n$ with exterior boundary ∂Y . The unit cells contain an evolving solid inclusion $Y_s(t) \subset Y$, and its complement, the evolving liquid part $Y_l(t) := Y \setminus \overline{Y_s(t)}$. Moreover, the solid–liquid interface Γ within the unit cell is defined by $\Gamma := \overline{Y_s} \cap \overline{Y_l}$.

In addition, we assume separation of scales. Let $\varepsilon \ll 1$ denote the scale parameter and presuppose that the macroscopic domain Ω_0 is an ideal porous medium: For the case $n = 3$ (and analogously for $n = 2$), it is given by the periodic composition of scaled and shifted unit cells $Y_\varepsilon^{i,j,k} := \varepsilon Y + \varepsilon(i, j, k)$ with $(i, j, k) \in \mathbb{Z}^3$. The scaled and shifted cells $Y_\varepsilon^{i,j,k}$, are divided into an analogously scaled liquid part $Y_{\varepsilon,l}^{i,j,k}(t)$ and solid part $Y_{\varepsilon,s}^{i,j,k}(t)$. The correspondingly scaled and shifted, solid–liquid interface is denoted by $\Gamma_\varepsilon^{i,j,k}(t)$. The liquid part of the domain Ω_0 is denoted by $\Omega_\varepsilon(t)$, its solid part $\Omega_0 \setminus \overline{\Omega_\varepsilon(t)}$, and the the solid–liquid interface, i.e. the interior boundary $\Gamma_\varepsilon(t)$ with unit outer normal ν_ε of the porous medium, are respectively defined by $\Omega_\varepsilon(t) := \bigcup_{i,j,k} Y_{\varepsilon,l}^{i,j,k}(t)$, $\Omega_0 \setminus \overline{\Omega_\varepsilon(t)} := \bigcup_{i,j,k} Y_{\varepsilon,s}^{i,j,k}(t)$, and

$\Gamma_\varepsilon(t) := \bigcup_{i,j,k} \Gamma_\varepsilon^{i,j,k}(t)$. The initial pore space is denoted by $\Omega_\varepsilon(0)$. Finally, the distribution of the solid and liquid phase and the solid–liquid interface are characterized by a level set function, cf. [32, 35]:

$$L_\varepsilon(t, x) \begin{cases} > 0 & \text{liquid phase } \Omega_\varepsilon(t), \\ = 0 & \text{interface } \Gamma_\varepsilon(t), \\ < 0 & \text{solid phase } \Omega \setminus \overline{\Omega_\varepsilon}(t). \end{cases} \tag{2.1}$$

We consider the following two- or three-dimensional pore-scale model for the description of diffusive transport within a porous medium $\Omega_\varepsilon(t)$; cf. [35] for the extension of our pore-scale model including fluid flow. In detail, we consider the transport equation (2.2a), in which c_ε denotes for the solute’s concentration and $d > 0$ its diffusivity. The level set equation (2.2e) for the level set L_ε characterizes the solid–liquid interface, cf. (2.1), which evolves in normal direction with velocity $v_{n,\varepsilon}$. For analytical investigations below, we restrict this general-level set approach to a simplified geometric setting.

At the evolving solid–liquid interface Γ_ε , the boundary condition (2.2b) is derived from mass conservation [35]. Supplementary, appropriate initial conditions c^0 (2.2d) and L^0 (2.2f) and, on the exterior boundary $\partial\Omega_0$, appropriate boundary conditions (2.2c) are chosen. In the following, the parameter ρ denotes the constant density of the solid. Finally, we summarize the pore-scale model:

$$\partial_t c_\varepsilon - \nabla \cdot (d \nabla c_\varepsilon) = 0 \qquad x \in \Omega_\varepsilon(t), \quad t \in (0, T), \tag{2.2a}$$

$$d \nabla c_\varepsilon \cdot \nu_\varepsilon = v_{n,\varepsilon} (c_\varepsilon - \rho) \qquad x \in \Gamma_\varepsilon(t), \quad t \in (0, T), \tag{2.2b}$$

$$c_\varepsilon(t, x) = 0 \qquad x \in \partial\Omega_0, \quad t \in (0, T), \tag{2.2c}$$

$$c_\varepsilon(0, x) = c^0(x) \qquad x \in \Omega_\varepsilon(0), \tag{2.2d}$$

$$\partial_t L_\varepsilon + v_{n,\varepsilon} |\nabla L_\varepsilon| = 0 \qquad x \in \Omega_0, \quad t \in (0, T), \tag{2.2e}$$

$$L_\varepsilon(0, x) = L^0(x) \qquad x \in \Omega_0. \tag{2.2f}$$

To close the system of model equations (2.2a)–(2.2f), a constitutive assumptions on the solid–liquid interface velocity $v_{n,\varepsilon}$ is required. Since we presuppose that the interface is evolving due to heterogeneous reactions f taking place at the solid–liquid interface Γ_ε , we directly relate the velocity $v_{n,\varepsilon}$ to the reaction f by

$$v_{n,\varepsilon} = \varepsilon \frac{1}{\rho} f(c_\varepsilon). \tag{2.2g}$$

Finally, only constitutive assumptions for the heterogeneous reaction rate f generating the evolution of the solid–liquid interface are required. In [35], a precipitation–dissolution rate is discussed with a quite general precipitation part of the reaction rate. The formulation of the dissolution part of the reaction rate by means of a Heaviside graph is standard and is motivated and used, e. g., in [11, 34]. Contrarily, we assume a linear precipitation rate f in this article which simplifies the model’s analysis in Section 4, since we hereby avoid higher than quadratic order non-linearities.

2.2 Effective model and its derivation

The main steps in deriving the effective model will be discussed at the end of this section after introducing the main technical tools for the purpose of upscaling in a level set framework. An extension of our effective model below, including fluid flow, was presented in [35] for two spatial dimensions. In the following, we define the two- or three-dimensional effective model (2.3)–(2.5), corresponding to the pore-scale model presented in Section 2.1:

$$\theta \partial_t c_0 - \nabla_x \cdot (\bar{D} \nabla_x c_0) = \sigma \frac{1}{\rho} f(c_0) c_0 - \sigma f(c_0) \quad \text{in } (0, T) \times \Omega_0, \tag{2.3a}$$

$$c_0(t, x) = 0 \quad \text{in } (0, T) \times \partial \Omega_0, \tag{2.3b}$$

$$c_0(0, x) = c^0(x) \quad \text{in } \Omega_0. \tag{2.3c}$$

$$\partial_t L_0 + \frac{1}{\rho} f(c_0) |\nabla_y L_0| = 0 \quad \text{in } (0, T) \times Y \times \Omega_0, \tag{2.3d}$$

$$L_0(0, x, y) = L^0(x, y) \quad \text{in } Y \times \Omega_0. \tag{2.3e}$$

For each $(t, x) \in (0, T) \times \Omega_0$, $Y_{l,0}(t, x) := \{y : L_0(t, x, y) > 0\}$, and $\Gamma_0(t, x) := \{y : L_0(t, x, y) = 0\}$. Moreover, $\theta := \frac{|Y_{l,0}|}{|Y|}$ and $\sigma := \frac{|\Gamma_0|}{|Y|}$ denote the porosity and specific surface, respectively. We emphasize here that θ is strictly positive and, contrary to the situation of rigid porous media, both θ and σ are functions of time and space. The diffusion tensor \bar{D} is defined by

$$\bar{D}_{ij} := \frac{1}{|Y|} \int_{Y_{l,0}(t,x)} d (\partial_{y_i} \zeta_j + \delta_{ij}) dy \tag{2.4}$$

and standard cell problems for ζ_j for $j = 1, 2, 3$ are given by

$$-\nabla_y \cdot (\nabla_y \zeta_j) = 0 \quad \text{in } Y_{l,0}(t, x), \tag{2.5a}$$

$$\nabla_y \zeta_j \cdot \nu_0 = -e_j \cdot \nu_0 \quad \text{on } \Gamma_0(t, x), \tag{2.5b}$$

$$\frac{1}{|Y|} \int_{Y_{l,0}(t,x)} \zeta_j dy = 0, \text{ and } \zeta_j \text{ is } Y\text{-periodic.} \tag{2.5c}$$

Under the assumption of linear precipitation, i.e. $f(c_0) = kc_0$, Equation (2.3a) simplifies to

$$\theta \partial_t c_0 - \nabla_x \cdot (\bar{D} \nabla_x c_0) = \sigma \frac{1}{\rho} k c_0^2 - \sigma k c_0 = \tilde{\tau} c_0^2 - \tilde{\sigma} c_0. \tag{2.6}$$

The coefficients $\tilde{\sigma} := \sigma k$ and $\tilde{\tau} := \tau k := \sigma \frac{k}{\rho}$ are related to the porosity θ by means of geometry. In particular, the specific surface σ can be expressed as a function $\sigma : (0, 1) \rightarrow \mathbb{R}$ depending on the porosity θ ; σ is non-negative and continuous in θ . If a parametrization of the underlying cell geometry by a single parameter is possible the relations are further discussed in Remark 2.2. A problem formulation involving (2.6) for such a simplified geometric setting is further analysed in Section 4.

Alternatively, it is reasonable to consider the re-scaling $\hat{c} := \theta c_0$ and state the following reformulation of the effective transport equation (2.3) for \hat{c} that reads

$$\partial_t \hat{c} - \nabla_x \cdot (\hat{D} \nabla_x \hat{c} - \hat{v} \hat{c}) = -\hat{k} \hat{c}$$

with $\hat{D} := \frac{\bar{D}}{\theta}$, $\hat{v} := \frac{\bar{D}}{\theta^2} \nabla_x \theta$, and $\hat{k} = \frac{\sigma}{\theta} k$. In general, the velocity \hat{v} is not divergence free and \hat{k} has dimension $1/T$, whereby $\frac{\sigma}{\theta}$ is the specific surface area related to the pore space instead of total volume.

We now comment on the upscaling of the pore-scale model (2.2a)–(2.2g). To that end, we first revise the method of two-scale asymptotic expansion in a level set framework, cf. [35], and point out its extension to the three-dimensional setting. Thereafter, this method is applied to equations (2.2a)–(2.2g). Distinctions between the three-dimensional derivations and the two-dimensional case are highlighted.

Owing to the separation of scales, in addition to the global variable x , a microscopic variable y is introduced. Both variables are connected via the relation $y = x/\varepsilon$. As a consequence, the expansions of the gradient and further spatial derivatives read

$$\nabla = \nabla_x + \frac{1}{\varepsilon} \nabla_y, \quad \nabla \cdot = \nabla_x \cdot + \frac{1}{\varepsilon} \nabla_y \cdot, \quad \Delta = \Delta_x + 2 \frac{1}{\varepsilon} \nabla_x \cdot \nabla_y + \frac{1}{\varepsilon^2} \Delta_y. \tag{2.7a}$$

Furthermore, it is assumed that the concentration c_ε may be expanded in series of the scale parameter ε , i. e.

$$c_\varepsilon(t, x) = c_0(t, x, y) + \varepsilon c_1(t, x, y) + \varepsilon^2 c_2(t, x, y) + \dots, \quad y = x/\varepsilon. \tag{2.7b}$$

In addition to the expansions (2.7), in the framework of an evolving porous media, also the level set function L_ε itself and the outer normal vector v_ε must be expanded. In general, the expansion of the normal vector v_ε may be expressed in terms of the level set function L_ε , cf. [35]:

$$L_\varepsilon(t, x) = L_0(t, x, y) + \varepsilon L_1(t, x, y) + \varepsilon^2 L_2(t, x, y) + \dots, \quad y = x/\varepsilon, \tag{2.8a}$$

$$v_\varepsilon = v_0 + \varepsilon v_1 + O(\varepsilon^2), \tag{2.8b}$$

$$v_0 = \frac{\nabla_y L_0}{|\nabla_y L_0|}, \quad v_1 = \frac{\nabla_x L_0 + \nabla_y L_1}{|\nabla_y L_0|} - \frac{\nabla_x L_0 \cdot \nabla_y L_0}{|\nabla_y L_0|^2} v_0 - \frac{v_0 \cdot \nabla_y L_1}{|\nabla_y L_0|} v_0. \tag{2.8c}$$

In two dimensions, with the definition of $\tau_0 := v_0^\perp$ denoting the unit tangent on Γ_0 , the representation $v_1 = \tau_0 \frac{\tau_0 \cdot (\nabla_x L_0 + \nabla_y L_1)}{|\nabla_y L_0|}$ holds true, cf. [35]. However, such a expression may not be derived directly for the three-dimensional setting. This explicit representation is, however, only relevant for the formulation of [35, Lemma 3.2.], which up to now has been the basis for the purpose of upscaling in a level set framework. We extend the theory of [35] by establishing quite analogously to the derivations in [35] new versions of [35, Lemma 3.1.] and [35, Lemma 3.2.] for three dimensions. Later on, these new formulations will be applied to our pore-scale model (2.2a)–(2.2g). Thereby, $F := d(\nabla_x c_0 + \nabla_y c_1)$ and $g = F \cdot v_0$ are chosen in the context of Lemmas 2 and 1, respectively.

Lemma 1 *Let $g(t, x, y)$ be a scalar function such that $g(t, x, y) = 0$ for $y \in \Gamma_0(t, x)$, $x \in \Omega_0$, and $t \geq 0$. Then, for $y \in \Gamma_0(t, x)$, $x \in \Omega_0$, $t \geq 0$, it holds that*

$$\nabla_x g = \frac{v_0 \cdot \nabla_y g}{|\nabla_y L_0|} \nabla_x L_0.$$

[35, Lemma 3.1] and its proof directly transfer to the three-dimensional case as does [35, Lemma 3.2]. However, the result has to be reformulated without using the tangent vector τ_0 , which is not unique in three dimensions. We state this reformulation of in [35, Lemma 3.2] in the following and highlight the crucial steps in its proof.

Lemma 2 *Let $F(t, x, y)$ be a vector-valued function such that $\nabla_y \cdot F(t, x, y) = 0$ on $Y_0(t, x) := \{y | L_0(t, x, y) < 0\}$ and $v_0 \cdot F(t, x, y) = 0$ on $\Gamma_0(t, x)$ for $x \in \Omega_0$, and $t \geq 0$. Then, for $y \in \Gamma_0(t, x)$, $x \in \Omega_0$, $t \geq 0$, it holds that*

$$\int_{\Gamma_0(t,x)} \left(\frac{\nabla_y L_1}{|\nabla_y L_0|} - \frac{v_0 \cdot \nabla_y L_1}{|\nabla_y L_0|} v_0 \right) \cdot F - \frac{L_1}{|\nabla_y L_0|} v_0 \cdot \nabla_y (v_0 \cdot F) \, do_y = 0.$$

Proof The proof of Lemma 2 directly follows the lines of the proof in [35] by considering the right derivative (denoted by ∂_δ^+) of the integrals $\int_{Y_\pm^\delta} \nabla_y \cdot F dy$ with respect to $\delta > 0$, where $Y_\pm^\delta(t, x) := \{y | L_0(t, x, y) + \delta [L_1]_\pm(t, x, y) < 0\}$. Therefore, in three dimensions, we carefully evaluate the following expression:

$$\begin{aligned} & \int_{[0,1]^2} (\partial_\delta v^\delta|_{\delta=0} \cdot F + \nabla_y (v_0 \cdot F) \cdot \partial_\delta k_+|_{\delta=0}) |\det((D_s k_+)^T (D_s k_+))(s, 0)|^{\frac{1}{2}} \, ds \\ & = \partial_\delta \int_{Y_+^\delta} \nabla_y \cdot F dy|_{\delta=0} = 0, \end{aligned}$$

where $k_+(\cdot, 0) : [0, 1]^2 \rightarrow \Gamma_+^\delta := \{y | L_0 + \delta [L_1]_+ = 0\}$ parametrizes the interface Γ_+^δ of Y_+^δ . To this end, we consider the normal on Γ_+^δ which we denote by v^δ . We expand v^δ via

$$v^\delta = v_0 + \delta v_1^\delta + \dots$$

with $v_0 = \frac{\nabla_y L_0}{|\nabla_y L_0|}$ being the normal corresponding to L_0 . Moreover, we have the representation

$$v^\delta = \frac{\nabla_y (L_0 + \delta [L_1]_+)}{|\nabla_y (L_0 + \delta [L_1]_+)|}$$

which, by applying Taylor’s series, reads

$$v^\delta = \frac{\nabla_y L_0}{|\nabla_y L_0|} + \left(\frac{Id |\nabla_y L_0|^2 - \nabla_y L_0 \otimes \nabla_y L_0}{|\nabla_y L_0|^3} \right) \delta \nabla_y [L_1]_+ + \dots$$

We aim to determine $\partial_\delta v^\delta|_{\delta=0} = v_1^\delta$ and considering the calculations above, we obtain

$$\partial_\delta v^\delta|_{\delta=0} = \frac{\nabla_y[L_1]_+}{|\nabla_y L_0|} - \frac{v_0 \cdot \nabla_y[L_1]_+}{|\nabla_y L_0|} v_0.$$

All further investigations follow directly the lines in [35]. □

Remark 2.1 *In two dimensions, the above expression may be reformulated using the tangent vector τ_0 as*

$$\partial_\delta v^\delta|_{\delta=0} = \frac{\tau_0 \cdot \nabla_y[L_1]_+}{|\nabla_y L_0|} \tau_0.$$

In deriving the effective model equations (2.3)–(2.5) in three dimensions, there are certain aspects we would like to highlight:

- (1) The zeroth-order expansion L_0 of the level set function characterizes the zeroth-order time evolving domain $Y_{l,0}(t, x) := \{y : L_0(t, x, y) > 0\}$ and interface $\Gamma_0(t, x) := \{y : L_0(t, x, y) = 0\}$, [35].
- (2) Lemmas 1 and 2 enter the upscaling procedure when analysing the zeroth-order terms (2.9) of the transport equation (2.2a). We deduce the changes in the proof that have to be done in the three-dimensional setting:

$$\partial_t c_0 - \nabla_x \cdot (d\nabla_x c_0 + d\nabla_y c_1) - \nabla_y \cdot (d\nabla_x c_1 + d\nabla_y c_2) = 0. \tag{2.9}$$

The corresponding boundary condition (2.2b) is of order ε^1 . Using the notation $\lambda = -\frac{L_1}{|\nabla_y L_0|} - \frac{y \cdot \nabla_x L_0}{|\nabla_y L_0|}$ and bearing in mind the additional terms that occur due to the evolving pore geometry [35], it reads

$$\begin{aligned} & (d\nabla_x c_1 + d\nabla_y c_2) \cdot v_0 + (d\nabla_x c_0 + d\nabla_y c_1) \cdot v_1 \\ & + y \cdot \nabla_x (d\nabla_x c_0 + d\nabla_y c_1) \cdot v_0 + \lambda v_0 \cdot \nabla_y (d\nabla_x c_0 + d\nabla_y c_1) \cdot v_0 = \frac{1}{\rho} f(c_0)(c_0 - \rho). \end{aligned}$$

Defining $F := d(\nabla_x c_0 + \nabla_y c_1)$, taking the mean $\frac{1}{|Y|} \int_{Y_l(t,x)} \cdot dy$ of (2.9) and applying the previously stated boundary condition, we obtain by the transport theorem for the diffusive term and Gauss' theorem for third term in (2.9)

$$\begin{aligned} & \frac{1}{|Y|} \int_{Y_l} \partial_t c_0 \, dy - \nabla_x \cdot \left(\frac{1}{|Y|} \int_{Y_l} (d\nabla_x c_0 + d\nabla_y c_1) \, dy \right) - \frac{1}{|Y|} \int_{\Gamma_0} \frac{\nabla_x L_0}{|\nabla_y L_0|} \cdot F \, d\sigma_y \\ & + \frac{1}{|Y|} \int_{\Gamma_0} F \cdot v_1 + y \cdot \nabla_x (F \cdot v_0) + \lambda v_0 \cdot \nabla_y (F \cdot v_0) = \frac{1}{|Y|} \int_{\Gamma_0} \frac{1}{\rho} f(c_0)(c_0 - \rho) \, d\sigma_y. \end{aligned}$$

Substituting $\lambda = -\frac{L_1}{|\nabla_y L_0|} - \frac{y \cdot \nabla_x L_0}{|\nabla_y L_0|}$ and defining $g = F \cdot v_0$, Lemma 1 applies directly, and certain terms are eliminated. By means of the boundary condition of order ε^0 , it holds $v_0 \cdot F = 0$ on $\Gamma_0(t, x)$ for $x \in \Omega_0$ and $t \geq 0$. With this property, (2.8c), and Lemma 2, further terms cancel. Finally, inserting the cell problems (2.5) and

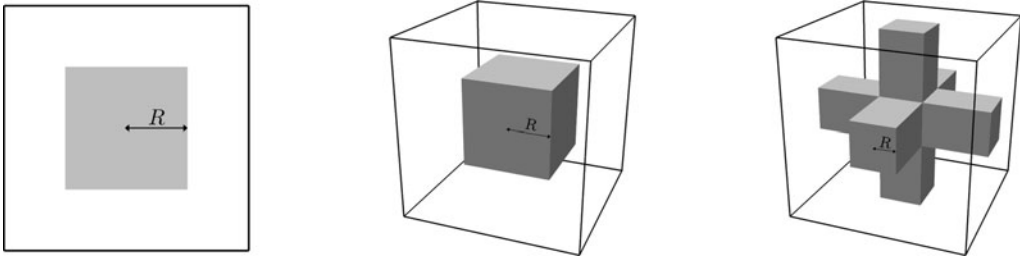


FIGURE 1. Examples for cell geometries: (a) two-dimensional square, (b) three-dimensional cube, (c) three-dimensional network.

the constitutive assumption on the velocity of the solid–liquid interface, we derive

$$\theta \partial_t c_0 - \nabla_x \cdot (\bar{D} \nabla_x c_0) = \frac{1}{|Y|} \int_{\Gamma_0(t,x)} \frac{1}{\rho} f(c_0)(c_0 - \rho) \, d\sigma_y = \sigma \frac{1}{\rho} f(c_0)c_0 - \sigma f(c_0).$$

2.3 Level set equation and geometry

Up to Section 2.2, the underlying microscopic geometry could have had quite arbitrary shape. We aim to have a geometry at hand that may be parametrized by a single parameter since it simplifies the investigation drastically in the following sense: As outlined below the level set equation which is an hyperbolic equation then reduces to an ODE. Instead of investigating the fully coupled PDE system (2.3)–(2.5), we restrict ourselves to a PDE–ODE system. We are well aware that this setting is simplified and idealized. However, on the other hand, it is numerically and analytically accessible and maintains the main difficulties and interesting aspects such as degenerating coefficients. Finally, the required assumptions on the geometry transfer directly to our assumption on the heterogeneous reaction rate since it dictates the behaviour of the geometry. We may interpret the situation as having local thermodynamic equilibrium or uniform precipitation preserving the geometric structure within a unit cell. However, the crucial part is that the reaction may nevertheless be x -dependent. This means that as time proceeds we have at best a locally periodic setting as in [37], even if starting with a periodic setting. As a remark note that under additional strong convection (which may be included in a straight forward way to our model), concentration gradients could be levelled out. This would simplify the situation drastically since it would lead to uniform precipitation within the whole macroscopic domain instead of a uniform precipitation within the unit cell.

The latter setting enables us to define a generalized “radius” R completely characterizing the geometrical setting. It is assumed that this parameter R changes uniformly within the cell, which yields y -independence of R from y . In this case, the hyperbolic level set equation (2.3d) reduces to an ODE for this “radius” R , see (2.10). According to the smooth relation between “radius” and porosity, (2.10) may be transformed to an ODE for the porosity, see (2.11).

For illustration, we consider that for every $t \in [0, T]$, the pore space and the corresponding boundary have shape (a), cf. Figure 1. However, further examples for

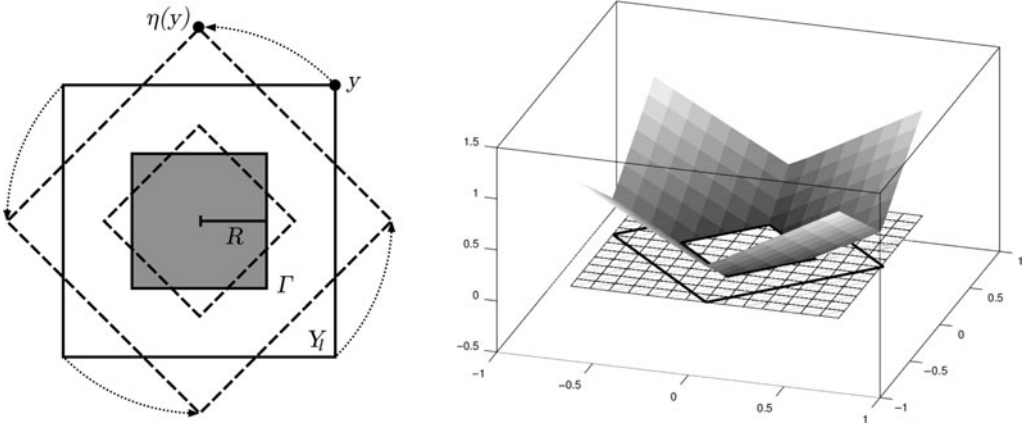


FIGURE 2. Visualization of the coordinate transformation $y \mapsto \eta(y)$ of the cell $Y = [-\frac{1}{2}, \frac{1}{2}]^2$ (left) and the transformed level set function $\tilde{L} = \tilde{L}(\eta)$ (right).

pore-scale geometries such as, e.g., shape (b) and (c), cf. Figure 1, and Y^1, Y^2, Y^3 , cf. Table 1, may be treated likewise to obtain (2.10). In the following, the single parameter $R(t, x) \in [0, \frac{1}{2}]$, $(t, x) \in (0, T) \times \Omega_0$, characterizes the evolution of these shapes:

- a) $Y_l(R(t, x)) := \{y \in [-\frac{1}{2}, \frac{1}{2}]^2 \mid R(t, x) < \|y\|_\infty < \frac{1}{2}\}$,
 $\Gamma(R(t, x)) := \{y \in [-\frac{1}{2}, \frac{1}{2}]^2 \mid \|y\|_\infty = R(t, x)\}$,
- b) $Y_l(R(t, x)) := \{y \in [-\frac{1}{2}, \frac{1}{2}]^3 \mid R(t, x) < \|y\|_\infty < \frac{1}{2}\}$,
 $\Gamma(R(t, x)) := \{y \in [-\frac{1}{2}, \frac{1}{2}]^3 \mid \|y\|_\infty = R(t, x)\}$,
- c) $Y_l(R(t, x)) := \{y \in [-\frac{1}{2}, \frac{1}{2}]^3 \mid R(t, x) < |y_i|, |y_j| < \frac{1}{2} \text{ for } i, j = 1, 2, 3, i \neq j\}$,
 $\Gamma(R(t, x)) := \{y \in [-\frac{1}{2}, \frac{1}{2}]^3 \mid |y_i| = R(t, x), |y_j| \leq R(t, x) \text{ and } |y_k| \geq R(t, x) \text{ for } i, j, k = 1, 2, 3, i \neq j \neq k \neq i\}$.

To derive the ODE that corresponds in case (a) to the level set equation (2.3d), we introduce new coordinates

$$\eta := \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}.$$

With respect to these coordinates, an appropriate level set function is defined by

$$\tilde{L}(\eta) := \begin{cases} \eta_2 + |\eta_1| - \sqrt{2}R & \text{if } \eta_2 \geq 0 \\ -\eta_2 + |\eta_1| - \sqrt{2}R & \text{if } \eta_2 < 0 \end{cases}$$

and the pore space can be rewritten as $Y_l(R) = \{\eta \in \mathbb{R}^2 \mid \|\eta\|_1 \in \sqrt{2}(R, 1/2)\}$. The coordinate transformation and the level set function \tilde{L} are visualized in Figure 2. Note

that \tilde{L} belongs to $C(Y_l(R)) \cap W^{1,\infty}(Y_l(R))$. This yields

$$\nabla_y L(y) = \frac{1}{\sqrt{2}} \nabla_\eta \tilde{L} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \frac{1}{\sqrt{2}} (1 - \operatorname{sgn} \eta_1, 1 + \operatorname{sgn} \eta_1).$$

Finally, taking the mean of equation (2.3d) indeed simplifies to the ODE

$$\partial_t R = \frac{1}{|Y|} \int_Y \frac{1 + |\operatorname{sgn} \eta_1|}{\sqrt{2}} \frac{1}{\rho} f(c_0) = \frac{1}{\rho} f(c_0). \tag{2.10}$$

Instead of the “radius” $R(t, x)$ of the grains we are more interested in the porosity $\theta(t, x)$ of the porous medium for each $(t, x) \in (0, T) \times \Omega_0$, which is nothing but the volume of $Y_l(R(t, x))$. The porosity θ depends smoothly on the “radius” R and vice versa. Furthermore, with Dirac delta δ and specific surface σ , the coarea formula yields the following relation describing the evolution of porosity

$$\partial_t \theta = -\frac{1}{\rho} f(c_0) \frac{1}{|Y|} \int_Y |\nabla_y L| \delta(L(t, x)) = -\frac{|L^{-1}(0)|}{|Y|} \frac{1}{\rho} f(c_0) = -\sigma(\theta) \frac{1}{\rho} f(c_0); \tag{2.11}$$

compare also the first term on the right-hand side of (2.3a). Consequently, the level set function, hence the evolution of the topology of the unit cell, is completely determined by the ODE for the porosity (2.11). In case of linear precipitation, i.e. $f(c_0) = kc_0$, it holds that

$$\partial_t \theta = -\sigma(\theta) \frac{k}{\rho} c_0. \tag{2.12}$$

Remark 2.2 *The specific surface σ describes the change of porosity θ with respect to radius R up to constants. Contrarily, R is related to θ , i.e. $|\Gamma(\theta)| = \sigma(\theta) = ((\frac{d}{dR}\theta) \circ R)(\theta)$, cf. (2.10) and (2.11). For instance, in case of shape (a) defined in Figure 1, we have $|\Gamma(\theta)| = 4\sqrt{1-\theta}$. Choosing instead the three-dimensional pendant (b) defined in Figure 1, we obtain $|\Gamma(\theta)| = 6\sqrt[3]{(1-\theta)^2}$. It is more challenging to describe a function σ as function of θ corresponding to shape (c) defined in Figure 1, but at least we easily have $|\Gamma(R(\theta))| = 48(\frac{1}{2} - R(\theta))R(\theta)$. However, since σ represents a polynomial with respect to the “radius” R , it holds that $\sigma : (0, 1) \rightarrow \mathbb{R}$ is a non-negative, smooth function with respect to θ provided this is also true for R .*

3 Cell problem and diffusion tensor

3.1 Analysis of the diffusion tensor

To analytically solve the cell problem

$$\begin{cases} -\Delta_y \zeta_j = 0 & \text{in } Y_l(\theta) \\ \nabla_y \zeta_j \cdot \nu = -e_j \cdot \nu \text{ on } \Gamma(\theta), \end{cases} \tag{3.1}$$

the interface $\Gamma(\theta)$ is not only assumed to evolve uniformly, cf. Section 2.3, but also to remain regular, i.e. $\Gamma(\theta)$ is a Lipschitz boundary. For illustration purposes, we are assuming in this section that the pore space $Y_l(\theta) := Y_l(R(\theta))$ is described by the three-dimensional

shape (c) defined in Figure 1. In the following, we are first interested in estimating the solutions of the cell problem. Second, we are interested in the smoothness properties of the diffusion coefficient $\bar{D} : [0, 1) \rightarrow \mathbb{R}^{3 \times 3}$ that depends on the porosity $\theta \in [0, 1)$ and is defined componentwise by

$$\bar{D}_{ij}(\theta) := \int_{Y_l(\theta)} d (\delta_{ij} + \partial_i \zeta_j(y)) \, dy \quad \text{if } \theta \in (0, 1)$$

and for vanishing porosity by $\bar{D}_{ij}(0) := 0$ for $i, j = 1, 2, 3$, cf. (2.4).

Similar to the approach in continuum mechanics and in [19], we first transform the given cell problems (3.1) into cell problems on the fixed geometry $Y_0 := Y_l(\frac{1}{2})$ via the map

$$\varphi^\theta : Y_l(\theta) \rightarrow Y_0, \quad \varphi^\theta(y) := \left[\left(\frac{1}{2 - 4R(\theta)} \left(|y_i| - \frac{1}{2} \right) + \frac{1}{2} \right) \cdot \text{sgn}(y_i) \right]_{i=1,2,3}.$$

We note that these transformations φ^θ belong to $C^\infty(Y_l(\theta))$ with the well-defined Jacobian $(J_y \varphi^\theta)(y) = \frac{1}{2 - 4R(\theta)} \mathbb{E}$ for $R(\theta) < \frac{1}{2}$. Let $a^\theta : H^1(Y_l(\theta)) \times H^1(Y_l(\theta)) \rightarrow \mathbb{R}$ denotes the bilinear form corresponding to the Laplacian on $Y_l(\theta)$. For all $u, v \in H^1(Y_l(\theta))$, there holds the equation

$$\begin{aligned} a^\theta(u, v) &:= \int_{Y_l(\theta)} \nabla_y u \cdot \nabla_y v = \int_{Y_l(\theta)} \nabla_y (\tilde{u} \circ \varphi^\theta) \cdot \nabla_y (\tilde{v} \circ \varphi^\theta) \\ &= \int_{Y_l(\theta)} \sum_{i=1}^3 \left(\sum_{k=1}^3 \partial_k \tilde{u} \partial_i \varphi_k^\theta \right) \left(\sum_{l=1}^3 \partial_l \tilde{v} \partial_i \varphi_l^\theta \right) \\ &= (2 - 4R(\theta))^{-2} \int_{Y_l(\theta)} (\nabla_{\tilde{y}} \tilde{u})(\varphi^\theta(y)) \cdot (\nabla_{\tilde{y}} \tilde{v})(\varphi^\theta(y)) \\ &= (2 - 4R(\theta))^{-2} \int_{Y_0} (\nabla_{\tilde{y}} \tilde{u})(\tilde{y}) \cdot (\nabla_{\tilde{y}} \tilde{v})(\tilde{y}) |\det(J_y \varphi^\theta)|^{-1} \\ &= (2 - 4R(\theta)) \int_{Y_0} \nabla_{\tilde{y}} \tilde{u} \cdot \nabla_{\tilde{y}} \tilde{v}, \end{aligned} \tag{3.2}$$

with $\tilde{u} := u \circ (\varphi^\theta)^{-1}$, $\tilde{v} := v \circ (\varphi^\theta)^{-1}$. Defining a matrix-valued function $A^\theta : Y_l(\theta) \rightarrow \mathbb{R}^{3 \times 3}$,

$$A_{kl}^\theta(\tilde{y}) := |\det(J_y \varphi^\theta)|^{-1} \sum_{i=1}^3 \partial_i \varphi_k^\theta(y) \partial_i \varphi_l^\theta(y) = \delta_{kl} (2 - 4R(\theta)),$$

we easily get the ellipticity of the operator \tilde{L}^θ defined by

$$\tilde{L}^\theta(\tilde{u}) := - \sum_{k,l=1}^3 A_{kl}^\theta(\partial_{kl} \tilde{u}) = -(2 - 4R(\theta)) \Delta_{\tilde{y}} \tilde{u}.$$

Due to (3.2), the weak solutions of the cell problems (3.1) are nothing but $\zeta_j := \tilde{\zeta}_j \circ \varphi^\theta \in H^1(Y_l(\theta))$, where $\tilde{\zeta}_j \in H^1(Y_0)$ are the weak solutions of the φ^θ -transformed cell

problems (3.3),

$$\begin{cases} \tilde{L}^\theta(\tilde{\zeta}_j) = 0 & \text{in } Y_0, \\ \nabla_{\tilde{y}} \tilde{\zeta}_j \cdot \nu_0 = -(2 - 4R(\theta))^2 e_j \cdot \nu_0 & \text{on } \Gamma_0, \end{cases} \tag{3.3}$$

whereby $\Gamma_0 := \Gamma(\frac{1}{2})$. These solutions $\tilde{\zeta}_j$ are unique up to a constant. Similarly, the diffusion tensor \bar{D} can be expressed by integrals over the fixed domain Y_0 via:

$$\begin{aligned} \bar{D}_{ij}(\theta) &= \int_{Y_i(\theta)} d(\delta_{ij} + \partial_i \zeta_j) = \int_{Y_i(\theta)} d \left(\delta_{ij} + \sum_{k=1}^3 (\partial_k \tilde{\zeta}_j)(\partial_i \varphi_k^\theta) \right) \\ &= \int_{Y_i(\theta)} d(\delta_{ij} + ((\nabla \tilde{\zeta}_j) \circ \varphi^\theta) \cdot \partial_i \varphi^\theta) \\ &= d(2 - 4R(\theta))^3 |Y_0| + d(2 - 4R(\theta))^2 \int_{Y_0} (\partial_i \tilde{\zeta}_j). \end{aligned}$$

Since we assume $R : [0, 1) \rightarrow (0, \frac{1}{2})$ to be smooth with respect to θ , the crucial term on the right-hand side investigating the smoothness of \bar{D} is the integral $\int_{Y_0} (\partial_i \tilde{\zeta}_j)$. This integral can be estimated by the H^1 -norm of $\tilde{\zeta}_j$. Furthermore, for all $\theta_1, \theta_2 \in (0, 1)$ and for the corresponding weak solutions $\tilde{\zeta}_j(\theta_1), \tilde{\zeta}_j(\theta_2)$ to (3.3), we may apply the elliptic theory to obtain the inequality

$$\begin{aligned} \int_{Y_0} |\partial_i \tilde{\zeta}_j(\theta_1) - \partial_i \tilde{\zeta}_j(\theta_2)| &\leq |Y_0|^{\frac{1}{2}} \|\tilde{\zeta}_j(\theta_1) - \tilde{\zeta}_j(\theta_2)\|_{H^1(Y_0)} \\ &\leq C |Y_0|^{\frac{1}{2}} \|e_j \cdot \nu_0\|_{L^2(\Gamma_0)} |R(\theta_1) - R(\theta_2)|^2. \end{aligned} \tag{3.4}$$

Since $2 - 4R(\theta)$ is constant with respect to \tilde{y} , the difference $\tilde{\zeta}_j(\theta_1) - \tilde{\zeta}_j(\theta_2)$ satisfies (in a weak sense) $\Delta_{\tilde{y}}(\tilde{\zeta}_j(\theta_1) - \tilde{\zeta}_j(\theta_2)) = 0$ in Y_0 . Hence, we obtain the continuity of the diffusion coefficient \bar{D} in $(0, 1)$. A similar estimate as in (3.4) yields the continuity in 0. Indeed the tensor \bar{D} belongs to $C^\infty([0, 1))$, since it inherits the regularity from the boundary condition (3.3). This can be illustrated for the first derivative $\bar{D}'(\theta)$ as follows: The unique solution of

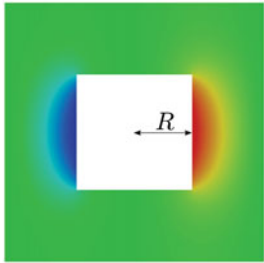
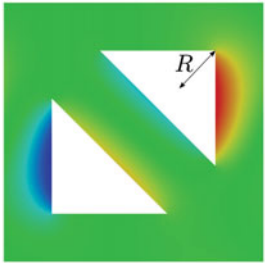
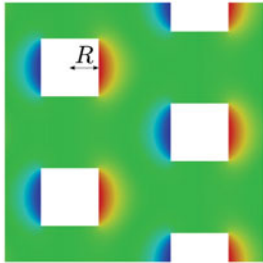

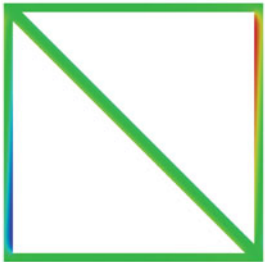
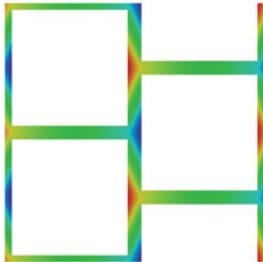
$$\begin{cases} \tilde{L}^\theta(\zeta'_j) = 0 & \text{in } Y_0 \\ \nabla_{\tilde{y}} \zeta'_j \cdot \nu_0 = 4(2 - 4R(\theta))R'(\theta)e_j \cdot \nu_0 & \text{on } \Gamma_0 \end{cases}$$

is nothing but the first derivative of $\tilde{\zeta}_j$ with respect to θ . Similar to (3.4), it holds

$$\begin{aligned} \int_{Y_0} |\partial_i(\zeta'_j(\theta_1) - \partial_i \zeta'_j(\theta_2))| &\leq |Y_0|^{\frac{1}{2}} \|\zeta'_j(\theta_1) - \zeta'_j(\theta_2)\|_{H^1(Y_0)} \\ &\leq C |Y_0|^{\frac{1}{2}} \|e_j \cdot \nu_0\|_{L^2(\Gamma_0)} [|R(\theta_1) - R(\theta_2)|R'(\theta_1)| + |R(\theta_2)|R'(\theta_1) - R'(\theta_2)] \end{aligned}$$

such that \bar{D} at least belongs to $C^1([0, 1))$. Moreover, the diffusion tensor \bar{D} is symmetric and positive definite for every $\theta \in (0, 1)$, cf. [25]. In case of “radially” uniform evolution of the microstructure, the diffusion tensor reduces to a scalar function $D(\theta) \geq 0$, i.e. $\bar{D}(\theta) = D(\theta)\mathbb{E}$ with unit matrix \mathbb{E} .

Table 1. Cell geometries and corresponding computed tensors, illustrated for the three considered families of cells Y^i , for porosities of $\theta = 0.8$ (top) and $\theta = 0.2$ (bottom)

Y^1	Y^2	Y^3
		
$\begin{bmatrix} 0.644 & 0.000 \\ 0.000 & 0.644 \end{bmatrix}$	$\begin{bmatrix} 0.605 & -0.079 \\ -0.079 & 0.605 \end{bmatrix}$	$\begin{bmatrix} 0.636 & 0.000 \\ 0.000 & 0.647 \end{bmatrix}$
		
$\begin{bmatrix} 0.109 & 0.000 \\ 0.000 & 0.109 \end{bmatrix}$	$\begin{bmatrix} 0.107 & -0.032 \\ -0.032 & 0.107 \end{bmatrix}$	$\begin{bmatrix} 0.091 & 0.000 \\ 0.000 & 0.109 \end{bmatrix}$

3.2 Numerical computations

We solve the cell problems (2.5) numerically in two space dimensions for three different (evolving) cell geometries and compute the corresponding effective diffusion tensors as defined in (2.4). The three different cells are denoted by $Y^i = Y^i(R)$, $i = 1, 2, 3$, each of which is linearly parametrized by a single parameter R . Table 1 illustrates the geometries of the fluid phases for porosity $\theta = 0.8$, which are possible initial configurations, and porosity $\theta = 0.2$, corresponding to configurations after a precipitation process has taken place.

The corresponding $j = 1, 2$ cell problems are solved using Raviart–Thomas elements of lowest order [23] on unstructured triangular meshes. In using mixed finite elements, the flux unknowns $\xi_j := -\nabla_y \zeta_j - e_j$, which have to be integrated for the computation of the diffusion tensor, are computed directly. For the computation of the functional relation between diffusion tensor and porosity, 100 sampling points are used on the porosity axis in Figure 3. The meshes on the representative unit cells contain between 30,000 and 70,000 triangles. Figure 3 illustrates the eigenvalues of the computed tensors on Y^i (for diagonal tensors, the eigenvalues equal the entries). In this way, the dependency of the diffusion tensor on the generalized “radius” R respectively on the porosity is highlighted: The functional relation as highlighted theoretically in Section 3.1 is smooth. Moreover, it is seen in Figure 3 that the diffusion tensor degenerates whenever the porosity tends to zero, i. e. in the case of total clogging. Consistently, the diffusion tensor is unity in case of vanishing microstructure, i. e. in the case of complete dissolution.

Explicit values of the diffusion tensor for porosities of $\theta = 0.2$ and $\theta = 0.8$ are stated in Table 1. Due to the isotropic geometry of the cell, the diffusion tensors reduce to

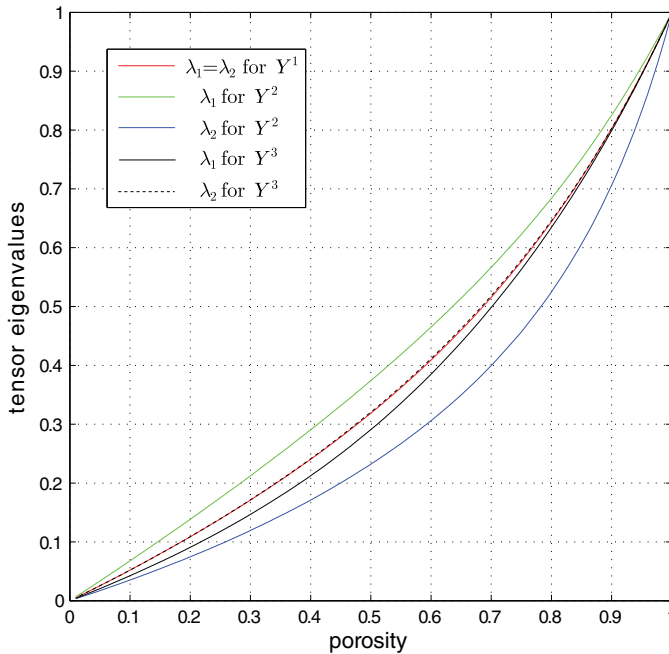


FIGURE 3. Functional relation between diffusion tensor’s eigenvalues λ_1, λ_2 and porosity, illustrated for the three considered families of cells Y^1, Y^2, Y^3 .

diagonal tensors $D(\theta)\mathbb{E}_2$ in the first setting, i.e. the tensors are in fact scalar coefficients. The second example accounts for anisotropic effects resulting in non-zero off-diagonal elements. Finally, in the third example, a diagonal matrix is again the result; this time with eigenvalues that do not coincide.

4 Analysis

In this section, we prove existence of solutions to the effective equations (2.3)–(2.3d) with general functions τ and σ . To this end, we apply Schauder’s fixed point theorem in strong solution spaces. Moreover, positivity of solutions and uniqueness is shown. Let us introduce the following notations: $\Omega_T := (0, T) \times \Omega$, $\partial\Omega_T := (0, T) \times \partial\Omega$, and $\|\cdot\|_p$ denoting the L^p -norm in Ω for $p \in [1, \infty]$. For the reader’s convenience, we restate the model equations under investigation in the following form (suppressing all indices etc.):

$$\theta \partial_t c - \nabla \cdot (D(\theta)\nabla c) = \tau(\theta)c^2 - \sigma(\theta)c \quad \text{in } \Omega_T, \tag{4.1a}$$

$$\partial_t \theta = -\tau(\theta)c \quad \text{in } \Omega_T, \tag{4.1b}$$

$$c(t, x) = 0 \quad \text{on } \partial\Omega_T, \tag{4.1c}$$

$$c(0, x) = c^0(x) \quad \text{in } \Omega, \tag{4.1d}$$

$$\theta(0, x) = \theta^0(x) \quad \text{in } \Omega. \tag{4.1e}$$

We denote the significant anisotropic Sobolev spaces by

$$\begin{aligned} \mathcal{X}_1 &:= W_r^{1,2}(\Omega_T) = L^r(0, T; W_r^2(\Omega)) \cap W_r^1(0, T; L^r(\Omega)), \\ \mathcal{X}_2 &:= W_r^{1-\frac{n}{2}, 2-\mu}(\Omega_T) = L^r(0, T; W_r^{2-\mu}(\Omega)) \cap W_r^{1-\frac{n}{2}}(0, T; L^r(\Omega)), \end{aligned}$$

where $r > n+2$ and $\mu > 0$ is assumed to be sufficiently small, i.e. $\mu < 1 - \frac{2+n}{r}$. In this case, \mathcal{X}_2 is compactly embedded in $W_{2r}^{\frac{3}{4}, \frac{3}{2}}(\Omega_T)$ as well as in $C^{\frac{1}{2}, 1}(\overline{\Omega_T})$, cf. [7, Theorem 2.2], [4].

Theorem 4.1 (Local in time existence of strong solutions) *Let $\Omega \subset \mathbb{R}^n$, $n = 2, 3$, be a domain with C^2 -smooth boundary $\partial\Omega$, $r > n + 2$, $c^0 \in W_r^{2-\frac{n}{2}}(\Omega)$, $c^0 \geq 0$, satisfying the compatibility condition $c^0|_{\partial\Omega} \equiv 0$ and $\theta^0 \in W_r^2(\Omega)$ with $\theta^0(x) \in (\delta, 1 - \delta) \subset (0, 1)$ for all $x \in \Omega$ and some $\delta \in (0, \frac{1}{2})$. Furthermore, let $D \in C^1((0, 1))$ be a positive scalar function and $\sigma \in C((0, 1))$, $\tau \in C^2((0, 1))$. Then, there exists a constant $T > 0$ and at least one strong solution $(c, \theta) \in \mathcal{X}_1^2$ solving (4.1).*

Proof First, we define the constants

$$\begin{aligned} \sigma_{\max} &:= \max_{\frac{\delta}{2} \leq \theta \leq 1 - \frac{\delta}{2}} \sigma(\theta), & \tau_{\max} &:= \max_{\frac{\delta}{2} \leq \theta \leq 1 - \frac{\delta}{2}} \tau(\theta), & D_{\max} &:= \max_{\frac{\delta}{2} \leq \theta \leq 1 - \frac{\delta}{2}} D(\theta), \\ \tau_{1,\max} &:= \max_{\frac{\delta}{2} \leq \theta \leq 1 - \frac{\delta}{2}} \tau'(\theta), & \tau_{2,\max} &:= \max_{\frac{\delta}{2} \leq \theta \leq 1 - \frac{\delta}{2}} \tau''(\theta), & D_{1,\max} &:= \max_{\frac{\delta}{2} \leq \theta \leq 1 - \frac{\delta}{2}} D'(\theta) \end{aligned}$$

and $D_{\min} := \min_{\frac{\delta}{2} \leq \theta \leq 1 - \frac{\delta}{2}} D(\theta) > 0$ limiting the corresponding functions. We further define the following non-empty, closed, and convex subset

$$\mathcal{K}_1 := \{c \in \mathcal{X}_1 : \|c\|_{\mathcal{X}_1} \leq K, \sup_{0 \leq t \leq T} \|c(t)\|_{2r} \leq 2\|c^0\|_{2r} \text{ and } \|\nabla c\|_{L^r(0,T;L^{2r}(\Omega))} \leq K^a\},$$

where $K \geq 1$ is assumed to be sufficiently large and $a \in (0, 1)$ is a suitable constant chosen below. Moreover, we set

$$\begin{aligned} \mathcal{K}_2 &:= \overline{\{c \in \mathcal{X}_2 : c \in \mathcal{K}_1\}}^{\|\cdot\|_{\mathcal{X}_2}}, \\ \mathcal{K}_3 &:= \{\theta \in \mathcal{X}_2 : \|\theta - \frac{1}{2}\|_{L^\infty(\Omega_T)} \leq K_\delta \text{ and } \sup_{0 \leq t \leq T} \|\nabla\theta(t)\|_{2r} \leq 2\|\nabla\theta^0\|_{2r}\} \end{aligned}$$

with $K_\delta := \frac{1}{2}(1 - \delta) < \frac{1}{2}$. We note that $c \in \mathcal{K}_2$ inherits the properties $\sup_{0 \leq t \leq T} \|c(t)\|_{2r} \leq 2\|c^0\|_{2r}$ and $\|\nabla c\|_{L^r(0,T;L^{2r}(\Omega))} \leq K^a$ from \mathcal{K}_1 . The fixed-point operator $\mathcal{F} : \mathcal{K}_1 \rightarrow \mathcal{K}_1$ is defined as the composition $\mathcal{F} := \mathcal{F}_2 \circ \mathcal{F}_1$ of $\mathcal{F}_1 : \mathcal{K}_1 \rightarrow \mathcal{K}_2 \times \mathcal{K}_3$ with $(\tilde{c}, \theta) := \mathcal{F}_1(\hat{c})$, whereby $\tilde{c} = \hat{c}$ and θ being the unique solution of the ODE

$$\partial_t \theta = -\tau(\theta)\hat{c} \tag{4.2}$$

and $\mathcal{F}_2 : \mathcal{K}_2 \times \mathcal{K}_3 \rightarrow \mathcal{K}_1$ with $c := \mathcal{F}_2(\tilde{c}, \theta)$ being the unique solution of the parabolic equation

$$\partial_t c - \nabla \cdot \left(\frac{D(\theta)}{\theta} \nabla c \right) = -\frac{\sigma(\theta)}{\theta} \tilde{c} + \frac{\tau(\theta)}{\theta} \tilde{c}^2 + \frac{D(\theta)}{\theta^2} \nabla \theta \cdot \nabla \tilde{c}. \tag{4.3}$$

\mathcal{F} is a well-defined self-map on \mathcal{K}_1 . Estimate (4.4) is obtained by Sobolev’s embedding theorem in space and Hölder’s inequality in time for all $c \in \mathcal{K}_1$ and will be used several times:

$$\int_0^T \|c(s)\|_{W^1_2(\Omega)} + \int_0^T \|c(s)\|_{W^\infty(\Omega)} \leq CT^{1-\frac{1}{r}} \|c\|_{L^r(0,T;W^2_r(\Omega))} \leq CKT^{1-\frac{1}{r}}, \tag{4.4}$$

where $C > 0$ is an appropriate constant.

Let $\hat{c} \in \mathcal{K}_1$. Since $\mathcal{X}_1 \subset \mathcal{X}_2$ and τ is Lipschitz continuous with respect to θ , there exists due to the existence theorem by Picard–Lindelöf, for all $x \in \Omega$, a unique solution $\theta(., x) \in C^1([0, T(x)])$, $T(x) > 0$, to the ODE

$$\partial_t \theta(., x) = -\tau(\theta(., x))\hat{c}(., x),$$

such that $\theta(t, x) \in (\frac{\delta}{2}, 1 - \frac{\delta}{2})$ for all $t \in [0, T(x)]$. Integration over time yields by means of (4.4)

$$\delta - \tau_{\max}CK \cdot T(x)^{1-\frac{1}{r}} \leq \theta(t, x) \leq 1 - \delta + \tau_{\max}CK \cdot T(x)^{1-\frac{1}{r}}.$$

We choose $T \in (0, 1)$ independently of x such that

$$\frac{\delta}{2} - \tau_{\max}CK \cdot T^{1-\frac{1}{r}} \geq 0, \tag{4.5}$$

i. e. $T^{1-\frac{1}{r}} \leq T_1(K)^{1-\frac{1}{r}} := \frac{\delta}{2\tau_{\max}CK}$. If we set $T(x) := T$ for all $x \in \Omega$, there holds $\|\theta - \frac{1}{2}\|_{L^\infty(\Omega_T)} \leq K_\delta$. So we obtain a unique solution $\theta \in C^1(0, T; L^\infty(\Omega))$ of the ODE (4.2). By testing the corresponding ODE

$$\partial_t(\partial_{x_i}\theta) = -(\partial_{x_i}(\tau \circ \theta))\hat{c} - \tau(\theta)\partial_{x_i}\hat{c} \tag{4.6}$$

for the spatial derivative $\partial_{x_i}\theta$, $i = 1, \dots, n$, with $|\partial_{x_i}\theta|^{2r-2}\partial_{x_i}\theta$, we have

$$\begin{aligned} \frac{1}{2r} \frac{d}{dt} \|\partial_{x_i}\theta(t)\|_{2r}^{2r} &= - \int_\Omega \tau'(\theta)\hat{c}|\partial_{x_i}\theta|^{2r} - \int_\Omega \tau(\theta)(\partial_{x_i}\hat{c})|\partial_{x_i}\theta|^{2r-2}\partial_{x_i}\theta \\ &\leq \tau_{1,\max}\|\hat{c}\|_\infty\|\partial_{x_i}\theta\|_{2r}^{2r} + \tau_{\max}\|\partial_{x_i}\hat{c}\|_{2r}\|\partial_{x_i}\theta\|_{2r}^{2r-1}. \end{aligned}$$

Gronwall’s Lemma (cf. Theorem A.1) together with (4.4) yields

$$\begin{aligned} \|\partial_{x_i}\theta(t)\|_{2r}^{2r} &\leq \left[\|\partial_{x_i}\theta^0\|_{2r} + \tau_{\max} \int_0^t \|\partial_{x_i}\hat{c}(t)\|_{2r} \right]^{2r} \exp\left(2r\tau_{1,\max} \int_0^t \|\hat{c}(t)\|_\infty\right) \\ &\leq \left[\|\partial_{x_i}\theta^0\|_{2r} + \tau_{\max}CKT^{1-\frac{1}{r}} \right]^{2r} e^{(2r\tau_{1,\max}CKT^{1-\frac{1}{r}})}. \end{aligned} \tag{4.7}$$

At this point, we require a further smallness property of T : Let $T \leq T_1(K)$ also satisfy $T^{1-\frac{1}{r}} \leq T_2(K)^{1-\frac{1}{r}} := \min\{\frac{\|\nabla\theta^0\|_{2r}}{2\tau_{\max}CK}, \frac{1}{4r^2\tau_{1,\max}CK}\}$. Since $\frac{3}{2}e^{1/2r} < 2$, it holds that due to the previous estimate

$$\sup_{0 \leq t \leq T} \|\nabla\theta(t)\|_{2r} \leq 2\|\nabla\theta^0\|_{2r} \tag{4.8}$$

holds. Testing the ODE

$$\partial_t(\partial_{x_j}\partial_{x_i}\theta) = (\partial_{x_j}\partial_{x_i}(\tau \circ \theta))\hat{c} - (\partial_{x_j}(\tau \circ \theta))(\partial_{x_i}\hat{c}) - (\partial_{x_i}(\tau \circ \theta))(\partial_{x_j}\hat{c}) - \tau(\theta)(\partial_{x_j}\partial_{x_i}\hat{c}) \quad (4.9)$$

which corresponds to the second-ordered derivative $\partial_{x_j}\partial_{x_i}\theta$, $i, j = 1, \dots, n$, with test function $|\partial_{x_j}\partial_{x_i}\theta|^{r-2}\partial_{x_j}\partial_{x_i}\theta$ yields $\theta \in \mathcal{X}_1$. Thus, the solution θ indeed belongs to \mathcal{K}_3 .

Now, consider the parabolic equation (4.3) for some $(\tilde{c}, \theta) \in \mathcal{F}_1(\mathcal{K}_1) \subseteq \mathcal{X}_1^2$. The regularity theorem (cf. Theorem A.2) for parabolic equations ensures the existence of a solution $c := \mathcal{F}_2(\tilde{c}, \theta)$ belonging to \mathcal{X}_1 . It remains to prove the self mapping property, i.e. $c \in \mathcal{K}_1$. To this end, testing (4.3) with $|c|^{2r-2}c$ yields similarly to (4.7)

$$\begin{aligned} \frac{1}{2r} \frac{d}{dt} \|c(t)\|_{2r}^{2r} + (2r - 1) \frac{D_{\min}}{1 - \frac{\delta}{2}} \|(c^{r-1}\nabla c)(t)\|_2^2 \\ \leq C'(\delta) (\|\tilde{c}\|_{2r} + \|\tilde{c}^2\|_{2r} + \|\nabla\theta\|_{2r}\|\nabla\tilde{c}\|_\infty) \|c\|_{2r}^{2r-1} \end{aligned} \quad (4.10)$$

with $C'(\delta) := \frac{4}{\delta^2}(\sigma_{\max} + \tau_{\max} + D_{\max})$. Applying Gronwall's Lemma (cf. Theorem A.1) as well as (4.4) leads to

$$\begin{aligned} \|c(t)\|_{2r}^{2r} &\leq \left[\|c^0\|_{2r} + 2C'(\delta) \left(\|c^0\|_{2r} \int_0^t (1 + \|\tilde{c}(t)\|_\infty) + \|\nabla\theta^0\|_{2r} \int_0^t \|\nabla\tilde{c}(t)\|_\infty \right) \right]^{2r} \\ &\leq \left[\|c^0\|_{2r} + 2C'(\delta) \left(\|c^0\|_{2r}T + (\|c^0\|_{2r} + \|\nabla\theta^0\|_{2r})CKT^{1-\frac{1}{r}} \right) \right]^{2r}. \end{aligned} \quad (4.11)$$

If necessary, we again reduce $T \leq \min\{T_1(K), T_2(K)\}$ such that

$$\sup_{0 \leq t \leq T} \|c(t)\|_{2r} \leq 2\|c^0\|_{2r}, \quad (4.12)$$

e.g. by choosing $T \leq T_0 := \frac{1}{4C'(\delta)}$ and $T^{1-\frac{1}{r}} \leq T_3^{1-\frac{1}{r}}(K) := \frac{\|c^0\|_{2r}}{4C'(\delta)(\|c^0\|_{2r} + \|\nabla\theta^0\|_{2r})CK}$. Moreover, by the regularity theory for parabolic equations (cf. Theorem A.2), we obtain the estimate

$$\begin{aligned} \|c\|_{\mathcal{X}_1} &\leq C_P \left(\|c^0\|_{W_r^{2-\frac{2}{r}}(\Omega)} + \left\| -\frac{\sigma(\theta)}{\theta}\tilde{c} + \frac{\tau(\theta)}{\theta}\tilde{c}^2 + \frac{D(\theta)}{\theta^2}\nabla\theta \cdot \nabla\tilde{c} \right\|_{L^r(\Omega_T)} \right) \\ &\leq C_P \left(\|c^0\|_{W_r^{2-\frac{2}{r}}(\Omega)} + 2C'(\delta) \left[\|c^0\|_{2r}T^{\frac{1}{r}}(|\Omega|^{\frac{1}{2r}} + 2\|c^0\|_{2r}) + \|\nabla\theta^0\|_{2r}K^a \right] \right) \\ &\leq K^{\frac{1+a}{2}} \leq K, \end{aligned} \quad (4.13)$$

if a constant $K := K(T_0, \|c^0\|_{W_r^{2-\frac{2}{r}}}, \|\nabla\theta^0\|_{2r}) \geq 1$ satisfies

$$\begin{aligned} K \geq \max \left\{ 1, \left(2C_P \left(\|c^0\|_{W_r^{2-\frac{2}{r}}(\Omega)} + 2C'(\delta)\|c^0\|_{2r}T_0^{\frac{1}{r}}(|\Omega|^{\frac{1}{2r}} + 2\|c^0\|_{2r}) \right) \right)^{\frac{2}{1+a}}, \right. \\ \left. \times (4C_P C'(\delta)\|\nabla\theta^0\|_{2r})^{\frac{2}{1+a}} \right\}. \end{aligned}$$

Finally, it remains to bound the norm $\|\nabla c\|_{L^r(0,T;L^{2r}(\Omega))}$ of the gradient to conclude $c \in \mathcal{K}_1$. Implying $r = 1$ in (4.10), we obtain for a constant $C_D := C_D(\delta, \|c^0\|_{2r}, \|\nabla\theta^0\|_{2r}) > 0$ by

means of the estimates (4.4), (4.8), and (4.12)

$$\int_0^t \|\nabla c\|_2^2 \leq \frac{2-\delta}{2D_{\min}} \left[\frac{1}{2} (\|c^0\|_2^2 - \|c\|_2^2) + C'(\delta) \int_0^t (\|\tilde{c}\|_2 + \|\tilde{c}^2\|_2 + \|\nabla\theta\|_2 \|\nabla\tilde{c}\|_\infty) \|c\|_2 \right] \leq C_D \left(1 + T + K T^{1-\frac{1}{r}} \right). \tag{4.14}$$

Moreover, testing (4.3) with $\partial_t c \in L^r(\Omega_T)$, integrating over time, and applying Young's inequality yields

$$\|\partial_t c\|_{L^2(\Omega_T)}^2 + \frac{D_{\min}}{1-\frac{\delta}{2}} \|\nabla c(t)\|_2^2 \leq \frac{2}{\delta} D_{\max} \|\nabla c^0\|_2^2 + \frac{4}{\delta^2} (D_{1,\max} + D_{\max}) \tau_{\max} \|\hat{c}|\nabla c|^2\|_{L^1(\Omega_T)} + C'(\delta) \left[C(\epsilon)(T|\Omega|)^{\frac{r-2}{r}} \|\tilde{c}\| + |\tilde{c}^2| + \|\nabla\theta\nabla\tilde{c}\|_{L^r(\Omega_T)}^2 + \epsilon \|\partial_t c\|_{L^2(\Omega_T)}^2 \right], \tag{4.15}$$

since there holds

$$-\int_\Omega \nabla \cdot \left(\frac{D(\theta)}{\theta} \nabla c \right) \partial_t c = \frac{1}{2} \frac{d}{dt} \int_\Omega \frac{D(\theta)}{\theta} |\nabla c|^2 - \frac{1}{2} \int_\Omega \left(\frac{D'(\theta)}{\theta} - \frac{D(\theta)}{\theta^2} \right) \partial_t \theta |\nabla c|^2.$$

Since the crucial terms of the right-hand side of (4.15) can be estimated by using the fact that $\hat{c} \in C^{\frac{1}{2},1}(\overline{\Omega_T})$ with a $\frac{1}{2}$ -Hölder constant $M > 0$ and applying (4.14), i.e.

$$\|\hat{c}|\nabla c|^2\|_{L^1(\Omega_T)} \leq \int_0^T \|\hat{c}(s) - \hat{c}(T)\|_\infty \|\nabla c(s)\|_2^2 ds + \int_0^T \|\hat{c}(T)\|_\infty \|\nabla c(s)\|_2^2 ds \leq C_D \left(1 + T + K T^{1-\frac{1}{r}} \right) \left(M T^{\frac{1}{2}} + K \right) \tag{4.16}$$

and by estimating in the same manner as in (4.13)

$$\|\tilde{c} + \tilde{c}^2 + \nabla\theta\nabla\tilde{c}\|_{L^r(\Omega_T)} \leq \left[\|c^0\|_{2r} T^{\frac{1}{r}} \left(|\Omega|^{\frac{1}{2r}} + 2\|c^0\|_{2r} \right) + \|\nabla\theta^0\|_{2r} K^a \right], \tag{4.17}$$

respectively, we are able to estimate $\|\nabla c\|_2$ in the L^r -norm with respect to time. There exist constants $C_D^{(i)} := C_D^{(i)}(\delta, \|c^0\|_{2r}, \|\nabla c^0\|_2, \|\nabla\theta^0\|_{2r}) > 0, i = 1, 2$, such that we obtain by combining (4.15), (4.16) as well as (4.17) and using (4.4)

$$\begin{aligned} \|\nabla c\|_{L^r((0,T);L^2(\Omega))}^r &\leq C_D^{(1)} + C_D^{(1)} \left(1 + T + K T^{1-\frac{1}{r}} \right)^{\frac{r}{2}} \left(T^{1+\frac{r}{4}} + T^{\frac{1}{2}} K^{\frac{r}{2}} \right) \\ &\quad + C_D^{(1)} T^{\frac{r}{2}} \left(T^{\frac{1}{2}} + K^{\frac{r}{2}a} \right)^2 \\ &\leq C_D^{(2)} \left(1 + T^{1+\frac{3}{4}r} + \left(T^{\frac{1}{2}} + T^{\frac{1}{2}+\frac{3}{4}r} \right) K^{\frac{r}{2}} + T^{\frac{r}{2}} K^r \right). \end{aligned}$$

Finally, we have for sufficiently large K and $a \in (\frac{1}{2}, 1)$ by reducing T ones again, i.e. choosing $T \leq T_4(K) := \frac{1}{K^{ra}} \leq 1$:

$$\|\nabla c\|_{L^r((0,T);L^2(\Omega))}^r \leq 5C_D^{(2)} K^{\frac{r}{4}} < C_S^{-2r^2(1-\frac{1}{2r})} K^{\frac{r}{2}a}, \tag{4.18}$$

where $C_S > 0$ denotes an adequate constant such that $\|u\|_{4r-2} \leq C_S \|u\|_{W^{1,r}(\Omega)}$ for all $u \in W_r^1(\Omega)$ by Sobolev's embedding theorem $W_r^1(\Omega) \hookrightarrow L^{4r-2}(\Omega)$. Hence, we obtain

by choosing $a := \frac{4r-2}{4r-1} \in (\frac{1}{2}, 1)$ and applying the interpolation inequality to time and space-dependent functions [7, Theorem 2.5], [3] $\left(\frac{1}{2r} = \frac{1}{2r} \cdot \frac{1}{2} + (1 - \frac{1}{2r})\frac{1}{4r-2}\right)$ the estimate

$$\begin{aligned} \|\nabla c\|_{L^r(0,T;L^{2r}(\Omega))} &\leq \|\nabla c\|_{L^r(0,T;L^2(\Omega))}^{\frac{1}{2r}} \|\nabla c\|_{L^r(0,T;L^{4r-2}(\Omega))}^{1-\frac{1}{2r}} \\ &\leq C_S^{1-\frac{1}{2r}} \|\nabla c\|_{L^r(0,T;L^2(\Omega))}^{\frac{1}{2r}} \|c\|_{\mathcal{X}_1}^{1-\frac{1}{2r}} \leq K^{\frac{a}{4r}} \cdot K^{(1-\frac{1}{2r})} = K^a. \end{aligned} \tag{4.19}$$

Due to (4.8), (4.12), (4.13), and (4.19), the operator $\mathcal{F} : \mathcal{K}_1 \rightarrow \mathcal{K}_1$ is a well-defined.

Continuity of the operator \mathcal{F} . To show continuity of \mathcal{F} , we first prove continuity of \mathcal{F}_1 . Therefore, let $(\hat{c}_k)_{k \in \mathbb{N}} \subset \mathcal{K}_1$ converge to $\hat{c} \in \mathcal{K}_1$. Then, the sequence $(\mathcal{F}_1(\hat{c}_k))_{k \in \mathbb{N}} =: ((\check{c}_k, \theta_k))_{k \in \mathbb{N}} \subset \mathcal{K}_2 \times \mathcal{K}_3$ converges to $\mathcal{F}_1(\hat{c}) =: (\check{c}, \theta) \in \mathcal{K}_2 \times \mathcal{K}_3$, since θ_k converges to θ in the $W_r^1((0, T); L^r(\Omega))$ -norm:

$$\begin{aligned} \frac{1}{r} \frac{d}{dt} \|\theta_k - \theta\|_r^r &= \int_{\Omega} |\tau(\theta_k)\hat{c}_k - \tau(\theta)\hat{c}| |\theta_k - \theta|^{r-1} \\ &\leq \tau_{1,\max} \|\hat{c}_k\|_{\infty} \|\theta_k - \theta\|_r^r + \tau_{\max} \|\hat{c}_k - \hat{c}\|_r \|\theta_k - \theta\|_r^{r-1}, \end{aligned}$$

which yields by Gronwall’s Lemma (cf. Theorem A.1)

$$\|\theta_k - \theta\|_r^r \leq \left[\tau_{\max} \int_0^t \|\hat{c}_k - \hat{c}\|_r \right]^r \exp\left(\tau_{1,\max} \int_0^t \|\hat{c}_k\|_{\infty} \right);$$

and further with (4.2)

$$\left\| \frac{d}{dt} \theta_k - \frac{d}{dt} \theta \right\|_r \leq \tau_{1,\max} \|\theta_k - \theta\|_r + \|\hat{c}_k - \hat{c}\|_r.$$

The convergence with respect to the $L^r((0, T); W_r^1(\Omega))$ -norm can be proven similarly, cf. (4.7). To extend convergence to the space $L^r((0, T); W_r^2(\Omega))$, we consider (4.9) and manage the first term on the right-hand side by using (4.8) and $\theta_k, \theta \in W_r^{1,1}(\Omega_T) \subset C^{0,0}(\overline{\Omega_T})$, i.e. $\sup_{(t,x) \in \Omega_T} |\tau''(\theta_k(t, x)) - \tau''(\theta(t, x))| \rightarrow 0$ if $k \rightarrow \infty$ since τ'' is uniformly continuous on $[\frac{\delta}{2}, 1 - \frac{\delta}{2}]$. Hence, even the slightly modified operator $\tilde{\mathcal{F}}_1 : \mathcal{K}_1 \rightarrow \mathcal{X}_1^2$, $\tilde{\mathcal{F}}_1(\hat{c}) := \mathcal{F}_1(\hat{c})$ (necessary for compactness below) is continuous.

To show continuity of \mathcal{F}_2 , let now $(\check{c}_k, \theta_k)_{k \in \mathbb{N}} \in \mathcal{K}_2 \times \mathcal{K}_3$ be an arbitrary sequence converging to $(\check{c}, \theta) \in \mathcal{K}_2 \times \mathcal{K}_3$ with respect to the \mathcal{X}_2 -norm. With $c_k := \mathcal{F}_2(\check{c}_k, \theta_k) \in \mathcal{X}_1$, $k \in \mathbb{N}$, and $c := \mathcal{F}_2(\check{c}, \theta) \in \mathcal{X}_1$, we set $\bar{c}_k := c_k - c$. The function \bar{c}_k solves the parabolic equation

$$\begin{aligned} \partial_t \bar{c}_k - \nabla \cdot \left(\frac{D(\theta_k)}{\theta_k} \nabla \bar{c}_k \right) &= -\frac{\sigma(\theta_k)}{\theta_k} \check{c}_k + \frac{\sigma(\theta)}{\theta} \check{c} + \frac{\tau(\theta_k)}{\theta_k} \check{c}_k^2 - \frac{\tau(\theta)}{\theta} \check{c}^2 + \frac{D(\theta_k)}{\theta_k^2} \nabla \theta_k \cdot \nabla \check{c}_k \\ &\quad - \frac{D(\theta)}{\theta^2} \nabla \theta \cdot \nabla \check{c} + \nabla \cdot \left(\left(\frac{D(\theta_k)}{\theta_k} - \frac{D(\theta)}{\theta} \right) \nabla c \right). \end{aligned}$$

However, solutions of this PDE fulfil the parabolic regularity estimate [7, Theorem 2.9]:

$$\begin{aligned}
 \|\tilde{c}\|_{\mathcal{X}_1} &\leq \left\| \frac{\sigma(\theta_k)}{\theta_k} - \frac{\sigma(\theta)}{\theta} \right\|_{L^\infty(\Omega_T)} \|\tilde{c}_k\|_{L^r(\Omega_T)} + \left\| \frac{\sigma(\theta)}{\theta} \right\|_{L^\infty(\Omega_T)} \|\tilde{c}_k - \tilde{c}\|_{L^r(\Omega_T)} \\
 &+ \left\| \frac{\tau(\theta_k)}{\theta_k} - \frac{\tau(\theta)}{\theta} \right\|_{L^\infty(\Omega_T)} \|\tilde{c}_k\|_{L^\infty(\Omega_T)} \|\tilde{c}_k\|_{L^r(\Omega_T)} \\
 &+ \left\| \frac{\tau(\theta)}{\theta} \right\|_{L^\infty(\Omega_T)} \|\tilde{c}_k + \tilde{c}\|_{L^\infty(\Omega_T)} \|\tilde{c}_k - \tilde{c}\|_{L^r(\Omega_T)} \\
 &+ \left\| \frac{D(\theta_k)}{\theta_k^2} - \frac{D(\theta)}{\theta^2} \right\|_{L^\infty(\Omega_T)} \|\nabla\theta_k\|_{L^{2r}(\Omega_T)} \|\nabla\tilde{c}_k\|_{L^{2r}(\Omega_T)} \\
 &+ \left\| \frac{D(\theta)}{\theta^2} \right\|_{L^\infty(\Omega_T)} \|\nabla\theta_k - \nabla\theta\|_{L^{2r}(\Omega_T)} \|\nabla\tilde{c}_k\|_{L^{2r}(\Omega_T)} \\
 &+ \left\| \frac{D(\theta)}{\theta^2} \right\|_{L^\infty(\Omega_T)} \|\nabla\theta\|_{L^{2r}(\Omega_T)} \|\nabla\tilde{c}_k - \nabla\tilde{c}\|_{L^{2r}(\Omega_T)} \\
 &+ \left\| \frac{D(\theta_k)}{\theta_k} - \frac{D(\theta)}{\theta} \right\|_{L^\infty(\Omega_T)} \|\Delta c\|_{L^r(\Omega_T)} \\
 &+ \left\| \frac{D'(\theta)\theta - D(\theta)}{\theta^2} \right\|_{L^\infty(\Omega_T)} \|\nabla\theta_k - \nabla\theta\|_{L^{2r}(\Omega_T)} \|\nabla c\|_{L^{2r}(\Omega_T)} \\
 &+ \left\| \frac{D'(\theta_k)\theta_k - D(\theta_k)}{\theta_k^2} - \frac{D'(\theta)\theta - D(\theta)}{\theta^2} \right\|_{L^\infty(\Omega_T)} \|\nabla\theta_k\|_{L^{2r}(\Omega_T)} \|\nabla c\|_{L^{2r}(\Omega_T)} \\
 &\leq \left(\left\| \frac{\sigma(\theta_k)}{\theta_k} - \frac{\sigma(\theta)}{\theta} \right\|_{L^\infty(\Omega_T)} + \left\| \frac{\tau(\theta_k)}{\theta_k} - \frac{\tau(\theta)}{\theta} \right\|_{L^\infty(\Omega_T)} + \left\| \frac{D(\theta_k)}{\theta_k^2} - \frac{D(\theta)}{\theta^2} \right\|_{L^\infty(\Omega_T)} \right. \\
 &\quad \left. + \left\| \frac{D(\theta_k)}{\theta_k} - \frac{D(\theta)}{\theta} \right\|_{L^\infty(\Omega_T)} + \left\| \frac{D'(\theta_k)\theta_k - D(\theta_k)}{\theta_k^2} - \frac{D'(\theta)\theta - D(\theta)}{\theta^2} \right\|_{L^\infty(\Omega_T)} \right) \\
 &\quad \times (\|\tilde{c}_k\|_{\mathcal{X}_2} + \|c\|_{\mathcal{X}_1})(1 + \|\tilde{c}_k\|_{\mathcal{X}_2} + \|\theta_k\|_{\mathcal{X}_2}) \\
 &\quad + \left(\frac{2\sigma_{\max}}{\delta} + 2\|\tilde{c}_k + \tilde{c}\|_{L^\infty(\Omega_T)} \frac{\tau_{\max}}{\delta} + \frac{4D_{\max}}{\delta^2} \|\theta\|_{\mathcal{X}_2} \right) \|\tilde{c}_k - \tilde{c}\|_{\mathcal{X}_2} \\
 &\quad + \left(\frac{4D_{\max}}{\delta^2} \|\tilde{c}_k\|_{\mathcal{X}_2} + 4 \frac{D_{1,\max}\theta_{0,\max} + D_{\max}}{\delta^2} \|c\|_{\mathcal{X}_1} \right) \|\theta_k - \theta\|_{\mathcal{X}_2}. \tag{4.20}
 \end{aligned}$$

Due to the uniform continuity of the functions σ, τ, D on $[\frac{\delta}{2}, 1 - \frac{\delta}{2}]$ and even of the derivative D' with respect to θ the sequence $(c_k)_{k \in \mathbb{N}}$ converges in \mathcal{X}_1 to c since we assumed the convergence of $(\tilde{c}_k, \theta_k)_{k \in \mathbb{N}}$ to (\tilde{c}, θ) in \mathcal{X}_2 , i.e. \mathcal{F} is a continuous map onto \mathcal{K}_1 .

Compactness of operator \mathcal{F} . Let $(\hat{c}_k)_{k \in \mathbb{N}} \subset \mathcal{K}_1$ be a bounded sequence. In particular, it holds $\|\hat{c}_k\|_{\mathcal{X}_1} \leq K$ for all $k \in \mathbb{N}$. Let $(\tilde{c}_k, \theta_k) := \mathcal{F}_1(\hat{c}_k) \in \mathcal{K}_2 \times \mathcal{K}_3$ be the corresponding images. Due to the compact embedding $\mathcal{X}_1 \subset\subset \mathcal{X}_2$, cf. [7, Theorem 2.2], the sequence $(\tilde{c}_k)_{k \in \mathbb{N}}$ is relatively compact. The relatively compactness of $(\theta_k)_{k \in \mathbb{N}}$ in \mathcal{X}_2 is given by the continuity of $\tilde{\mathcal{F}}_1 : \mathcal{K}_1 \rightarrow \mathcal{X}_1^2$, i.e. $(\theta_k)_{k \in \mathbb{N}}$ is bounded in \mathcal{X}_1 . Hence, the compactness of \mathcal{F}

is given by (4.20), since the images $c_k := \mathcal{F}_2(\tilde{c}_k, \theta_k)$ of a convergent subsequence denoted again by $(\tilde{c}_k, \theta_k)_{k \in \mathbb{N}}$ converge in \mathcal{K}_1 .

Existence of a fixed point. We proved in the previous steps that the operator \mathcal{F} is a continuous and compact self-map on a non-empty closed and convex set \mathcal{K}_1 . Thus, Schauder’s fixed point theorem yields at least one local-in-time strong solution. \square

Lemma 3 (Non-negativity) *Let the conditions of Theorem 4.1 be satisfied. Additionally, let σ and τ be non-negative functions. Then, the solution $(c, \theta) \in \mathcal{X}_1^2$ remains non-negative, i.e. $c(t, x) \geq 0$ and $\theta(t, x) > 0$ for all $(t, x) \in \Omega_T$.*

Proof Constructing the proof of Theorem 4.1, we immediately see that $\theta(t, x) \geq \frac{\delta}{2} > 0$. Let Ω^- be the support of $[c]_-$. To prove the non-negativity of c , we test (4.1a) with $-[c]_-$ and integrate over Ω^- to obtain

$$\frac{\delta}{4} \int_{\Omega^-} [c]_-^2(t) \leq \frac{1}{2} \int_{\Omega^-} \theta^0 [c]_-^2(0) - \int_0^t \int_{\Omega^-} \sigma(\theta) [c]_-^2 - \int_0^t \int_{\Omega^-} \tau(\theta) [c]_-^3 \leq 0.$$

Consequently, $\|[c]_-(t)\|_{L^2(\Omega^-)}^2 = 0$ for every t , i.e. $[c]_-(t, x) = 0$ for all $(t, x) \in (0, T) \times \Omega^-$ which implies $c(t, x) \geq 0$ for all $(t, x) \in \Omega_T$. \square

Theorem 4.2 (Uniqueness) *Let the conditions of Theorem 4.1 be satisfied. Additionally, let σ be a Lipschitz continuous function. Then, the strong solution $(c, \theta) \in \mathcal{X}_1^2$ to (4.1) is unique in \mathcal{X}_1^2 .*

Proof On the contrary, let us assume that additionally to the solution of problem (4.1) constructed in Theorem 4.1 $(c_1, \theta_1) \in \mathcal{X}_1^2$, there exists a solution called $(c_2, \theta_2) \in \mathcal{X}_1^2$. Let us first assume $\theta_2(t, x) \in [\frac{\delta}{2}, 1 - \frac{\delta}{2}]$ for all $(t, x) \in \Omega_T$, i.e. θ_2 also remains strictly positive. Setting $\bar{c} := c_1 - c_2$ and $\bar{\theta} := \theta_1 - \theta_2$ and subtracting the systems of equations satisfied by (c_1, θ_1) and (c_2, θ_2) gives

$$\begin{aligned} \partial_t \bar{c} - \nabla \cdot \left(\frac{D(\theta_1)}{\theta_1} \nabla \bar{c} \right) &= -\frac{\sigma(\theta_1)}{\theta_1} c_1 + \frac{\sigma(\theta_2)}{\theta_2} c_2 + \frac{\tau(\theta_1)}{\theta_1} c_1^2 - \frac{\tau(\theta_2)}{\theta_2} c_2^2 + \frac{D(\theta_1)}{\theta_1^2} \nabla \theta_1 \cdot \nabla c_1 \\ &\quad - \frac{D(\theta_2)}{\theta_2^2} \nabla \theta_2 \cdot \nabla c_2 + \nabla \cdot \left(\left(\frac{D(\theta_1)}{\theta_1} - \frac{D(\theta_2)}{\theta_2} \right) \nabla c_2 \right) \end{aligned} \tag{4.21a}$$

$$\partial_t \bar{\theta} = -(\tau(\theta_1) c_1 - \tau(\theta_2) c_2) \tag{4.21b}$$

in Ω_T with homogeneous initial data $\bar{c}(0) = \bar{\theta}(0) = 0$ as well as the homogeneous boundary condition $\bar{c} = 0$. Let L_σ, L_τ, L_D , and $L_{D,2}$ denote the Lipschitz constants of the maps $\frac{\sigma}{\theta}, \frac{\tau}{\theta}, \frac{D}{\theta}$, and $\frac{D}{\theta^2}$, respectively. We use $(\bar{c}, \bar{\theta})$ as the test function in the weak formulation of (4.21) to obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\bar{\theta}\|_2^2 &\leq \int_{\Omega} |\bar{\theta}| [|\tau(\theta_1)| |\bar{c}| + |c_2| |\tau(\theta_1) - \tau(\theta_2)|] \\ &\leq \frac{\tau_{\max}}{2} (\|\bar{c}\|_2^2 + \|\bar{\theta}\|_2^2) + \tau_{1,\max} \sup_{0 \leq t \leq T} \|c_2(t)\|_\infty \|\bar{\theta}\|_2^2 \end{aligned} \tag{4.22}$$

as well as

$$\begin{aligned}
 \frac{1}{2} \frac{d}{dt} \|\bar{c}\|_2^2 + \frac{D_{\min}}{1 - \frac{\delta}{2}} \|\nabla \bar{c}\|_2^2 &\leq \frac{2\sigma_{\max}}{\delta} \|\bar{c}\|_2^2 + \frac{L_\sigma}{2} \sup_{0 \leq t \leq T} \|c_2(t)\|_\infty (\|\bar{c}\|_2^2 + \|\bar{\theta}\|_2^2) \\
 &+ \frac{4\tau_{\max}}{\delta} \max_{i=1,2} \sup_{0 \leq t \leq T} \|c_i(t)\|_\infty \|\bar{c}\|_2^2 + \frac{L_\tau}{2} \left(\sup_{0 \leq t \leq T} \|c_2(t)\|_\infty \right)^2 (\|\bar{c}\|_2^2 + \|\bar{\theta}\|_2^2) \\
 &+ \frac{L_{D,2}}{2} \sup_{0 \leq t \leq T} \|\nabla \theta_1(t)\|_\infty \sup_{0 \leq t \leq T} \|\nabla c_1(t)\|_\infty (\|\bar{c}\|_2^2 + \|\bar{\theta}\|_2^2) \\
 &+ \frac{8D_{\max}}{\delta^2} \left(\sup_{0 \leq t \leq T} \|\nabla \theta_1(t)\|_\infty (C(\epsilon)\|\bar{c}\|_2^2 + \epsilon\|\nabla \bar{c}\|_2^2) \right. \\
 &\left. + \sup_{0 \leq t \leq T} \|\nabla c_2(t)\|_\infty (\|\bar{c}\|_2^2 + \|\nabla \bar{\theta}\|_2^2) \right) \\
 &+ \frac{L_D}{2} \sup_{0 \leq t \leq T} \|\nabla c_2\|_\infty (C(\epsilon)\|\bar{\theta}\|_2^2 + \epsilon\|\nabla \bar{c}\|_2^2), \tag{4.23}
 \end{aligned}$$

where $\epsilon > 0$ is chosen so small that the terms on the right-hand side of (4.23) dealing with $\nabla \bar{c}$ can be absorbed by diffusion term. Due to the last term of inequality (4.23), we also need an estimate for $\nabla \bar{\theta}$. Since $\nabla \bar{\theta}$ satisfies the ODE

$$\partial_t(\nabla \bar{\theta}) = -(\tau'(\theta_1)c_1\nabla \theta_1 - \tau'(\theta_2)c_2\nabla \theta_2 + \tau(\theta_1)\nabla c_1 - \tau(\theta_2)\nabla c_2),$$

we obtain by testing this ODE with $\nabla \bar{\theta}$ similarly to the previous estimates

$$\begin{aligned}
 \frac{1}{2} \frac{d}{dt} \|\nabla \bar{\theta}\|_2^2 &\leq \frac{\tau_{2,\max}}{2} \sup_{0 \leq t \leq T} \|c_1(t)\|_\infty \sup_{0 \leq t \leq T} \|\nabla \theta_1(t)\|_\infty (\|\nabla \bar{\theta}\|_2^2 + \|\bar{\theta}\|_2^2) \\
 &+ \frac{\tau_{1,\max}}{2} \sup_{0 \leq t \leq T} \|\nabla \theta_1(t)\|_\infty (\|\nabla \bar{\theta}\|_2^2 + \|\bar{c}\|_2^2) + \tau_{1,\max} \sup_{0 \leq t \leq T} \|c_2(t)\|_\infty \|\nabla \bar{\theta}\|_2^2 \\
 &+ \frac{\tau_{1,\max}}{2} \sup_{0 \leq t \leq T} \|\nabla c_1(t)\|_\infty (\|\nabla \bar{\theta}\|_2^2 + \|\bar{\theta}\|_2^2) + \frac{\tau_{\max}}{2} (C(\epsilon)\|\nabla \bar{\theta}\|_2^2 + \epsilon\|\nabla \bar{c}\|_2^2). \tag{4.24}
 \end{aligned}$$

We add (4.22)—(4.24). Then, for the function $\mathcal{B}(\bar{c}, \bar{\theta}) := \frac{1}{2}(\|\bar{c}\|_2^2 + \|\bar{\theta}\|_2^2 + \|\nabla \bar{\theta}\|_2^2)$ it holds

$$\frac{d}{dt} \mathcal{B}(\bar{c}, \bar{\theta}) \leq \Psi(t)\mathcal{B}(\bar{c}, \bar{\theta}) \quad \text{for a.e. } t \in (0, T),$$

where Ψ is a non-negative measurable function in t . By Gronwall’s inequality, $\mathcal{B}(\bar{c}, \bar{\theta}) = 0$ for a.e. t which implies $\|\bar{c}\|_2^2 + \|\bar{\theta}\|_2^2 = 0$. This shows that the solution (c, θ) exists uniquely.

Let us now suppose $\inf_{0 \leq t \leq T} \|\theta_2(t)\|_\infty < \frac{\delta}{2}$. Since $\theta_2 \in \mathcal{X}_1 \hookrightarrow C^{\frac{1}{2},1}(\Omega_T)$, there exists $T_1 \in (0, T)$ such that $\inf_{0 \leq t \leq T_1} \|\theta_2(t)\|_\infty \in (\frac{\delta}{4}, \frac{\delta}{2})$. Applying the preceding proof of uniqueness on the time interval $(0, T_1)$ yields equality of the solutions (c_1, θ_1) and (c_2, θ_2) in $(0, T_1) \times \Omega$. But $\inf_{0 \leq t \leq T_1} \|\theta_2(t)\|_\infty = \inf_{0 \leq t \leq T_1} \|\theta_1(t)\|_\infty \geq \frac{\delta}{2}$ contradicts the supposition. We argue in the same manner to assure $\sup_{0 \leq t \leq T} \|\theta_2(t)\|_\infty \leq 1 - \frac{\delta}{2}$. \square

Due to (4.5), (4.8), (4.12), and (4.18), the existence interval $(0, T)$ of the unique solution $(c, \theta) \in \mathcal{X}_1^2$ to (4.1) can even be estimated from below by

$$T \geq \min\{T_0, T_1(K), T_2(K), T_3(K), T_4(K)\}.$$

The next result states extensibility of the existence interval of the strong solution to (4.1) until the phenomena of pore-clogging appears at time $T_{\text{clog}} > 0$. This can directly be proven under the assumption of more regularity on the data since the property $\sup_{0 \leq t \leq T} \|c(t)\|_{W_r^{2-2/r}(\Omega)} < \infty$ for all $T < T_{\text{clog}}$ is needed.

Corollary 1 (Solvability up to clogging) *Let the conditions of Theorems 4.1, 4.2, and Lemma 3 be satisfied with the additional regularity assumptions $c^0 \in W_r^{4-2/r}(\Omega)$, $\theta^0 \in W_r^{3-2/r}(\Omega)$, $D \in C^3((0, 1))$ and $\sigma \in C^2((0, 1))$. Suppose also the compatibility conditions $(\nabla\theta^0 \cdot \nabla c^0)|_{\partial\Omega} \equiv 0$ and $\Delta c^0|_{\partial\Omega} \equiv 0$. Moreover, let $(0, T)$ be the maximal existence interval of the unique non-negative solution (c, θ) of (4.1) belonging to \mathcal{X}_1^2 with $\theta(t, x) \in (0, 1)$ for all $(t, x) \in (0, T) \times \Omega$, i.e. (c, θ) can not be extended to a non-negative solution $(\tilde{c}, \tilde{\theta}) \in W_r^{1,2}((0, \tilde{T}) \times \Omega)$ for some $\tilde{T} > T$. Then, there holds either*

$$\liminf_{t \nearrow T} \inf_{x \in \Omega} \theta(t, x) = 0 \quad \text{or} \quad T = \infty.$$

Proof Let us suppose $T < \infty$ and there exists $\delta' \in (0, \frac{1}{2})$ such that $\inf_{x \in \Omega} \theta(t, x) \geq \delta'$ for all $t \in (0, T)$, where $(0, T)$ denotes the maximal existence interval of the solution $(c, \theta) \in \mathcal{X}_1^2$. We obtain with (4.7) and (4.11)

$$\sup_{0 \leq t \leq T} \|c(t)\|_{2r} + \sup_{0 \leq t \leq T} \|\nabla\theta(t)\|_{2r} < \infty.$$

We consider the PDE

$$\begin{aligned} \theta \partial_t c' - \nabla \cdot (D(\theta)\nabla c') &= (3\tau(\theta)c - \sigma(\theta))c' - \tau'(\theta)\tau(\theta)c^3 + \sigma'(\theta)\tau(\theta)c^2 \\ &\quad - \nabla \cdot (D'(\theta)\tau(\theta)c\nabla c) && \text{in } \Omega_T \\ c'(t, x) &= 0 && \text{on } \partial\Omega_T \\ c'(0) &= \frac{1}{\theta^0} [\tau(\theta^0)(c^0)^2 - \sigma(\theta^0)c^0 + \nabla \cdot (D(\theta^0)\nabla c^0)] && \text{in } \Omega. \end{aligned}$$

corresponding to $c' := \partial_t c$ with $c'(0) \in W_r^{2-\frac{2}{r}}(\Omega)$. In the same way as in (4.13) of the proof of Theorem 4.1, we conclude $c' \in W_r^{1,2}(\Omega_T) \subset C(\overline{\Omega_T})$. Since c satisfies the elliptic equation

$$-\nabla \cdot (D(\theta)\nabla c) = \tau(\theta)c^2 - \sigma(\theta)c - \theta \partial_t c$$

for each fixed $t \in (0, T)$ elliptic L^p -regularity theory [9] yields

$$\|D^2 c\|_r \leq C \|\tau(\theta)c^2 - \sigma(\theta)c - \theta \partial_t c\|_r + \|c\|_2$$

and hence $\sup_{0 \leq t \leq T} \|c(t)\|_{W_r^2(\Omega)} < \infty$. We even obtain $c \in C(0, T; W_r^{2-\frac{2}{r}}(\Omega))$ by Aubin–Lions compactness lemma.

We now set $\tilde{T} := \min\{\tilde{T}_0, \tilde{T}_1(\tilde{K}), \tilde{T}_2(\tilde{K}), \tilde{T}_3(\tilde{K}), \tilde{T}_4(\tilde{K})\} > 0$, where \tilde{K} and \tilde{T}_i , $i = 0, \dots, 3$, denotes the modified constants K and T_i introduced in the proof of Theorem 4.1 by replacing δ , $\|c^0\|_{2r}$, $\|\nabla\theta^0\|_{2r}$ and $\|c^0\|_{W_r^{2-2/r}(\Omega)}$ with the bounds δ' , $\sup_{0 \leq t \leq T} \|c(t)\|_{2r}$, $\sup_{0 \leq t \leq T} \|\nabla\theta(t)\|_{2r}$ and $\sup_{0 \leq t \leq T} \|c(t)\|_{W_r^{2-2/r}(\Omega)}$, respectively. Furthermore, let $\tilde{t} := T -$

$\tilde{T}/2$. Then, Theorem 4.1 yields a strong solution $(\tilde{c}, \tilde{\theta})$ on $(\tilde{t}, \tilde{t} + \tilde{T})$ with initial data $(c(\tilde{t}), \theta(\tilde{t}))$ which coincides by Theorem 4.2 with (c, θ) on $(0, T)$, i.e. (c, θ) can be extended to $(0, T + \tilde{T}/2)$. This contradicts the assumption on $(0, T)$ being the maximal existence interval. \square

Remark 4.1 For the previous result, it suffices to assume the weakened additional integrability assumptions $c^0 \in W_\kappa^{4-2/\kappa}(\Omega)$, $\theta^0 \in W_\kappa^{3-2/\kappa}(\Omega)$ with $\kappa > 1 + \frac{n}{2}$. With such a choice of κ , the inclusion $W_\kappa^{1,2}(\Omega_T) \subset C(\overline{\Omega_T})$ holds. Moreover, we obtain by parabolic regularity theory (cf. Theorem A.2) $c' \in W_\kappa^{1,2}(\Omega_T)$. In contrast to (4.13) in the proof of Theorem 4.1, the corresponding norm must not be estimated by a constant K and thus there is no need for the solution to belong to $C^{\frac{1}{2},1}(\overline{\Omega_T})$.

In either case, there holds the embedding $W_\kappa^{3-\frac{2}{\kappa}}(\Omega) \subset C^1(\overline{\Omega})$. Thus, the restriction $\nabla\theta^0|_{\partial\Omega}$ to the boundary $\partial\Omega$ is reasonable to ensure that the compatibility condition is well-defined.

Let $n = 2$ and $r = 2$. Suppose we have a local-in-time strong solution $c, \theta \in W_2^{1,2}(\Omega_T)$ for example, by regularizing a weak solution. The extension of this solution up to clogging at $T_{\text{clog}} > 0$ could be done without additional assumptions on the data since due to the embedding $W^{1,2}(0, T; L^2(\Omega)) \cap L^2(0, T; W^{2,2}(\Omega)) \subset C(0, T; W^{1,2}(\Omega))$ there already holds $\sup_{0 \leq t \leq T} \|c(t)\|_{W_2^1(\Omega)} < \infty$ for all $T < T_{\text{clog}}$.

5 Conclusion

We investigated a diffusion–precipitation model in an evolving porous medium. Its up-scaling was performed and the resulting model was analysed. In detail, we first generalized the method of two-scale asymptotic expansion in a level set framework [35] for three spatial dimensions. Applying this method to the diffusion–precipitation model, an upscaled, quadratically non-linear diffusion equation with effective, time- and space-dependent coefficients was obtained. The regularity of these coefficients was analysed and possible degeneration of the diffusion tensor with respect to porosity was illustrated by numerical simulations.

The second major aspect of this work was the analysis of the non-linear PDE coupled to an ODE. We proved positivity, existence, and uniqueness of a strong solution up to a possible clogging phenomena by applying Schauder’s fixed point theorem. In this respect, the obtained results extend the understanding of diffusion–precipitation models presented in or based on [11, 35].

A limitation of our work that could easily be overcome, is the restriction to a single parameter. More general or complex geometries being described by several independent parameters would lead to a system of ODEs in the respective parameters. Such a situation can be analysed along the same lines as in Sections 3 and 4. Considering the full PDE–PDE problem (including the level-set equation) instead needs different analytical tools.

A further limitation of our analysis is the fact that we did not include the dissolution process to our analysis. This could introduce further complications as it is commonly modelled by a Heaviside graph which is a multi-valued function [10, 34]. To handle the multi-valuedness, a regularization of the Heaviside graph must be performed. The main issue in using the regularization technique is obtaining *a-priori* estimates that are

independent of the regularization parameter with the help of which the author passes to the limit as the regularization parameter tends to zero. Contrary to our investigations, applying this approach additionally to evolving porous media seems reasonable for defining solutions in a weaker space, e. g. $c(t) \in W^{1,r}(\Omega)$ for a.e. t .

Further work needs to be undertaken to extend our findings to the case of several mobile and immobile species being present in an evolving porous medium. In [12], multi-species, diffusion–reaction-systems including non-linear, homogeneous reactions following the mass action law are investigated and the existence of a unique, positive, and global strong solution is shown in appropriate function spaces.

Combining all these approaches would likely be a reasonable way to tackle comprehensive diffusion–precipitation–reaction systems in evolving porous media.

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Appendix A

A.1 Variables and parameters

Here, L denotes a characteristic length, T a characteristic time, and N the amount of a substance.

\cdot^0		physical quantity of order ε^0
\cdot^0		initial values
\cdot^ε		physical quantity on pore-scale
$\bar{\cdot}$		y -averaged physical quantity
$[\cdot]^\pm$		positive/negative part of \cdot , i.e. $\cdot = [\cdot]_+ - [\cdot]_-$
∇	$1/L$	gradient
∂_t	$1/T$	time derivative
c	N/L^3	concentration
d	L^2/T	diffusivity in the fluid
\bar{D}	L^2/T	diffusion tensor
D	L^2/T	scalar diffusion
δ_{ij}	–	Kronecker delta
e_j	–	j th unit vector
ε	–	scale parameter, ratio of pore size to domain size
f	$N/L^2/T$	surface reaction rate
Γ	L^2	solid–liquid interface
Γ_0	L^2	solid–liquid interface within unit cell
Γ_ε	L^2	interior boundary of Ω_ε
$\Gamma_\varepsilon^{i,j,k}$	L^2	solid–liquid interface within scaled unit cell
k	L/T	rate coefficient
\hat{k}	$1/T$	rate coefficient
L	–	level set function
ν	–	outer unit normal
Ω	L^3	global domain
$\partial\Omega$	L^2	exterior boundary
Ω_ε	L^3	periodic, perforated domain
R	L	parametrization of geometry
ρ	N/L^3	density of the solid phase
σ	$1/L$	specific surface area
t	T	time
τ		rescaled specific surface area
$\theta = Y_l / Y $	–	water content = porosity
v_n	L/T	normal velocity of the solid–liquid interface
x	L	global space variable
y	L	microscopic space variable
Y	L^3	unit cell
$Y_\varepsilon^{i,j,k}$	L^3	scaled unit cell
Y_l	L^3	fluid phase within unit cell
$Y_{l,0}$	L^3	fluid phase within unit cell
$Y_{l,\varepsilon}^{i,j,k}$	L^3	fluid phase within scaled unit cell
Y_s	L^3	solid phase within unit cell
$Y_{s,\varepsilon}^{i,j,k}$	L^3	solid phase within scaled unit cell

A.2 Inequalities and theorems

Theorem A.1 (Gronwall’s inequality [33]). *Let F_1 and F_2 be non-negative and integrable functions on $[0, T]$ and let $\gamma \in (0, 1)$ as well as $C > 0$ be constants. Assume that the function $f \in C([0, T])$ satisfies*

$$f(t) \leq C + \int_0^t F_1(s)f(s)^{1-\gamma} ds + \int_0^t F_2(s)f(s) ds$$

for all $t \in [0, T]$. Then, the inequality

$$f(t) \leq \left[C^\gamma + \gamma \int_0^t F_1(s) ds \right]^{\frac{1}{\gamma}} \exp \left(\int_0^t F_2(s) ds \right)$$

holds for all $t \in [0, T]$.

Theorem A.2 (Parabolic regularity theory [7, Theorem 2.9]). *Suppose $\Omega \subset \mathbb{R}^n$ is a domain with C^2 -smooth boundary $\partial\Omega$, $\frac{3}{2} \neq r > 1$, A is a bounded and elliptic tensor whose coefficients belong to $C^0(\Omega_T) \cap L^s(0, T; W^1_s(\Omega))$ with $s > \max(r, n + 2)$. Suppose $f \in L^r(\Omega_T)$, $u_0 \in W^{2-\frac{2}{r}}_r(\Omega)$, and $U_0 \in W^{1-\frac{1}{(2r)}, \frac{2-1}{r}}_r(\partial\Omega_T)$. In the case of $r > \frac{3}{2}$, let the initial and boundary data be compatible in the sense $U_0(0, \cdot) = u_0$ on $\partial\Omega$. Then, the solution u of*

$$\begin{aligned} \partial_t u - \nabla \cdot (A \nabla u) &= f && \text{in } \Omega_T \\ u &= U_0 && \text{on } \partial\Omega_T \\ u(0, \cdot) &= u_0 && \text{in } \Omega \end{aligned}$$

is an element of $W^{1,2}_r(\Omega_T)$ and satisfies the a priori estimate

$$\|u\|_{W^{1,2}_r(\Omega_T)} \leq C \left(\|f\|_{L^r(\Omega_T)} + \|U_0\|_{W^{1-\frac{1}{(2r)}, \frac{2-1}{r}}_r(\partial\Omega_T)} + \|u_0\|_{W^{2-\frac{2}{r}}_r(\Omega)} \right)$$

with a constant C independent of f , U_0 , and u_0 .