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A homogenisation-based two-scale model for reactive transport in media with evolving microstructure

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Abstract

A two-scale model for reactive transport in a porous medium with an evolving phase configuration is formulated. The model equations are derived from a pore-scale model by homogenisation and are defined on a time-dependent geometry. Two different settings are considered: In the first one, an evolving pore-water distribution is a-priori given. In the second one, the pore water evolves due to the reaction itself. By transforming the system to a reference configuration, it can be proven that both settings lead to mathematically well-posed problems. ***To cite this article: S. Meier, C. R. Mecanique 336 (2008).***
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Résumé

Sur un système de réaction–diffusion à deux échelles avec une évolution de la micro-structure. On propose un modèle à deux échelles pour décrire le transport réactif dans des milieux poreux, dont la micro-structure change dans le temps. Les équations du modèle sont définies dans une géométrie spatiale qui dépend du temps et elles sont obtenues a partir d'un modèle microscopique par la méthode d'homogénéisation. Deux situations différentes sont considérés : Dans le premier cas, une évolution de la distribution de l'eau de pores est donnée a priori. Dans le deuxième cas, c'est bien la réaction qui cause l'évolution de l'eau. En outilisant un changement des systèmes de coordonnées, on prouve que les deux situations conduisent à des problèmes qui sont mathématiquement bien posés. ***Pour citer cet article : S. Meier, C. R. Mecanique 336 (2008).***
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Keywords: Porous media; Homogenisation; Reaction–diffusion; Multiscale approach

Mots-clés : Milieux poreux ; Homogénéisation ; Réaction et diffusion ; Approche multiéchelle

1. Introduction

Transport processes in media with a highly complex and varying microstructure occurs in a variety of situations in technical, biological or geological applications. In this work, a two-scale model is presented in order to accurately model a reaction–diffusion process in a porous medium involving highly different time scales. For the special case of constant and periodic microstructure, the two-scale concept is well-known, for instance as a model for flow in fissured

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media [1–3]. It is mathematically justified by periodic homogenisation [4,5]. However, in general the multiple phases in a porous medium evolve in time. Important examples are air–water systems in unsaturated soils or the porous matrix of concrete, which grows due to precipitation of reaction products. Obviously, such changes can have an influence on the size and connectivity of the pore channels and, consequently, affect the transport velocity and need to be modelled.

Homogenisation with evolving microstructure has been encountered in the literature in at least two different ways: The first solution consists in describing the time-dependent interfaces between the phases either by a level set [6] or by a smooth phase-field approximation [7]. In both cases, the balance equations for the concentrations can be rewritten as PDEs with periodic coefficients on the whole of Ω. The second approach consists in transforming the equations to a fixed periodic reference geometry by a (virtual) deformation [8–10], similar as done in continuum mechanics. The first approach is more suitable for numerical simulations. The second approach, however, turns out to be very useful for obtaining analytical results, even though the transformed PDEs are more complicated than the original ones. The main drawback – besides a considerable technical effort – is that topology changes have to be excluded at present.

The second approach has been worked out for the evolution of the *solid* phase in a porous medium. In this work, we follow similar ideas in order to construct a mathematical framework for two-scale reaction–diffusion models including an evolving *liquid* phase. It is important to note that this evolution in time needs *not* to be periodic and is restricted only by the assumption that the connectivity of the different phases remains invariant in time. Two conceptually different scenarios are distinguished:

(i) The evolution is independent of the reaction–diffusion process and can be considered as *a-priori given*.
(ii) The evolution is caused by the reaction–diffusion process via production of water. In this case, a *coupled* model is needed.

The model problem considered throughout this work is a simplified version of a reaction–diffusion system modelling a chemical degradation process in concrete structures. For details on this real-world application, we refer to [11–13]. The complete analysis including all proofs can be found in [14] and will be presented in forthcoming publications.

2. Microscopic model with evolving geometry

Let $\Omega \subset \mathbb{R}^n$ be some region occupied by the porous medium. For any time $t > 0$, let Ω be decomposed into subdomains $\overline{\Omega} = \overline{\Omega}_{\mathrm{s}}^{\varepsilon}(t) \cup \overline{\Omega}_{\mathrm{l}}^{\varepsilon}(t) \cup \overline{\Omega}_{\mathrm{g}}^{\varepsilon}(t)$, where $\Omega_{\mathrm{s}}^{\varepsilon}(t)$, $\Omega_{\mathrm{l}}^{\varepsilon}(t)$ and $\Omega_{\mathrm{g}}^{\varepsilon}(t)$ are disjoint domains occupied by the solid, liquid and gaseous phase, respectively. The quantity $\varepsilon > 0$ is a typical length scale of the microstructure. The *internal boundaries* or *interfaces* are denoted by:

$$S_{\mathrm{lg}}^{\varepsilon}(t) := \partial\Omega_{\mathrm{l}}^{\varepsilon}(t) \cap \partial\Omega_{\mathrm{g}}^{\varepsilon}(t), \qquad S_{\mathrm{ls}}^{\varepsilon}(t) := \partial\Omega_{\mathrm{l}}^{\varepsilon}(t) \cap \partial\Omega_{\mathrm{s}}^{\varepsilon}(t), \qquad S_{\mathrm{gs}}^{\varepsilon}(t) := \partial\Omega_{\mathrm{g}}^{\varepsilon}(t) \cap \partial\Omega_{\mathrm{s}}^{\varepsilon}(t)$$

For $\alpha, \beta \in \{\mathrm{s}, \mathrm{l}, \mathrm{g}\}$, $\alpha \neq \beta$, let $\nu_{\alpha\beta}^{\varepsilon}(t,x)$ be the unit normal at the point $x \in S_{\alpha\beta}^{\varepsilon}(t)$, directed towards the β-phase. Moreover, let $w_{\alpha\beta}^{\varepsilon}(t,x)$ be the normal velocity of the interface $S_{\alpha\beta}^{\varepsilon}(t)$. Note that, in general, the *exterior boundary* $\Gamma := \partial\Omega$ also splits up into three time-dependent parts, namely:

$$\Gamma = \big(\Gamma \cap \overline{\Omega}_{\mathrm{g}}^{\varepsilon}(t)\big) \cup \big(\Gamma \cap \overline{\Omega}_{\mathrm{l}}^{\varepsilon}(t)\big) \cup \big(\Gamma \cap \overline{\Omega}_{\mathrm{s}}^{\varepsilon}(t)\big)$$

We consider now a substance A that is present in the gaseous phase as a gas with concentration $c_1^{\varepsilon}(t,x)$ and in the liquid phase as a solute with concentration $c_2^{\varepsilon}(t,x)$. The concentrations are re-scaled by the (dimensionless) Henry constant $H > 0$, such that their equilibrium is given by $c_1^{\varepsilon} = c_2^{\varepsilon}$. In the liquid phase, A takes part in a chemical reaction with rate $\eta(c_2^{\varepsilon}) \geqslant 0$. The diffusivity $\hat{D}_2 > 0$ of A in the liquid phase is assumed much slower than that in the gaseous phase (D_1) and is therefore re-scaled as $\hat{D}_2 = \varepsilon^2 D_2$. As in the well-known case of a constant and periodic geometry, this specific scaling causes the homogenisation procedure to result in a two-scale model. The mass balance of A is then given by the system:

$$\partial_t c_1^{\varepsilon} - \operatorname{div}(D_1 \nabla c_1^{\varepsilon}) = 0 \quad \text{in } \Omega_{\mathrm{g}}^{\varepsilon}(t) \tag{1a}$$

$$\partial_t c_2^{\varepsilon} - \operatorname{div}(\varepsilon^2 D_2 \nabla c_2^{\varepsilon}) + \eta(c_2^{\varepsilon}) = 0 \quad \text{in } \Omega_{\mathrm{l}}^{\varepsilon}(t) \tag{1b}$$

$$H^{-1}(-D_1 \nabla c_1^{\varepsilon} \cdot \nu_{\mathrm{lg}}^{\varepsilon} - c_1^{\varepsilon} w_{\mathrm{lg}}^{\varepsilon}) = -\varepsilon^2 D_2 \nabla c_2^{\varepsilon} \cdot \nu_{\mathrm{lg}}^{\varepsilon} - c_2^{\varepsilon} w_{\mathrm{lg}}^{\varepsilon} \quad \text{on } S_{\mathrm{lg}}^{\varepsilon}(t) \tag{1c}$$

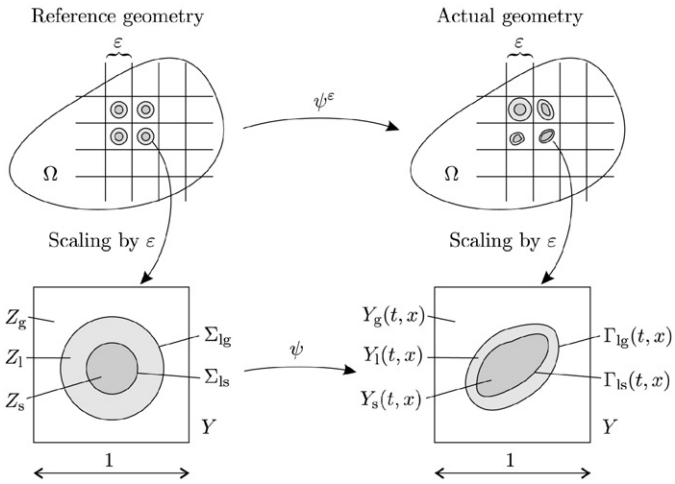

Fig. 1. Transformation of the time-dependent geometry to a periodic reference configuration.

For the second interfacial condition, we account for three different types of kinetics. They distinguish in the occurrence of additional flux terms. Using Kronecker symbols $\delta_{ii} := 1$ and $\delta_{ij} := 0$ if $i \neq j$, the three cases[1] $j \in \{2, 3, 4\}$ can be written simultaneously as:

$$-\varepsilon^2 D_2 \nabla c_2^\varepsilon \cdot \nu_{\mathrm{lg}}^\varepsilon - c_2^\varepsilon w_{\mathrm{lg}}^\varepsilon = \varepsilon k_2 (c_2^\varepsilon - c_1^\varepsilon) - \delta_{j2} c_2^\varepsilon w_{\mathrm{lg}}^\varepsilon - \delta_{j3} H^{-1} c_1^\varepsilon w_{\mathrm{lg}}^\varepsilon \quad \text{on } S_{\mathrm{lg}}^\varepsilon(t) \tag{1d}$$

Here $k_2 > 0$ is some exchange coefficient. At the external boundary, we impose a Robin condition for A in the gaseous phase,

$$-D_1 \nabla c_1^\varepsilon \cdot \nu_\Gamma = b_1 (c_1^\varepsilon - c_1^{\mathrm{ext}}) \quad \text{on } \Gamma \cap \overline{\Omega_{\mathrm{g}}^\varepsilon}(t) \tag{1e}$$

where $b_1 > 0$ is another exchange coefficient and $c_1^{\mathrm{ext}}(t)$ is a given ambient concentration. On the remaining boundaries and interfaces, exchange of A is not allowed and the corresponding fluxes are zero. After adding appropriate initial conditions, (1) yields a closed system for determining the unknown concentrations c_1^ε and c_2^ε. We refer to it by **Problem ($\mathbf{M}_\psi^\varepsilon$)**.

3. The two-scale limit model

The following analysis can be regarded as a generalisation of the one-dimensional analysis presented in [15]. It is based on an assumption on the evolving geometry.

Assumption A. The actual pore geometry is the image of an ε-periodic reference geometry by a time-dependent one-to-one transformation, which is assumed a-priori known.

To be more precise, assume we are given a partition of the unit cube $Y := (0, 1)^n$ into disjoint subdomains:

$$\overline{Y} = \overline{Z_{\mathrm{s}} \cup Z_{\mathrm{l}} \cup Z_{\mathrm{g}}}$$

See also Fig. 1. The periodic reference domains are defined via:

$$G_\alpha^\varepsilon(t) := \mathrm{int}\left(\Omega \cap \bigcup_{k \in \mathbb{Z}^n} \varepsilon (k + \overline{Z}_\alpha) \right), \quad \alpha \in \{\mathrm{s}, \mathrm{l}, \mathrm{g}\}$$

where $\mathrm{int}(G)$ denotes the interior of a domain G. This reference geometry is transformed to the actual, time-dependent (non-periodic) geometry by means of a coordinate transformation ψ^ε acting one-to-one in the settings:

$$\psi^\varepsilon(t, \cdot) : G_\alpha^\varepsilon(t) \to \Omega_\alpha^\varepsilon(t), \quad y = \psi^\varepsilon(t, z) \quad \text{for each } \alpha \in \{\mathrm{s}, \mathrm{l}, \mathrm{g}\}$$

[1] The case $j = 1$ corresponds to the Dirichlet condition $c_1^\varepsilon = c_2^\varepsilon$ (cf. [14]) and is not treated in this paper.

We assume the following asymptotic expansion to be valid for the transformation:

$$\psi^\varepsilon(t,x) = x + \varepsilon\psi^0\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon^2\psi^1\left(t,x,\frac{x}{\varepsilon}\right) + \cdots$$

where the coefficient functions $\psi^i(t,x,z)$, $i \in \mathbb{N}$, are Y-periodic with respect to the variable z. Then the first-order approximations of the geometry are:

$$Y^0_\alpha(t,x) := \psi^0(t,x,Z_\alpha), \qquad \Gamma^0_{\alpha\beta}(t,x) := \psi^0(t,x,\Sigma_{\alpha\beta})$$

Let $\nu^0_{\alpha\beta}$ and $w^0_{\alpha\beta}$ be the unit normal and normal velocity at $\Gamma^0_{\alpha\beta}$. If we assume $\nu^\varepsilon(t,x) \approx \nu^0(t,x,x/\varepsilon)$, then $w^\varepsilon_{\alpha\beta}$ is related to $w^0_{\alpha\beta}$ via:

$$\begin{aligned} w^\varepsilon_{\alpha\beta}(t,x) &= \partial_t\psi^\varepsilon(t,x)\cdot\nu^\varepsilon_{\alpha\beta}(t,x) \\ &\approx \varepsilon\partial_t\psi^0(t,x,x/\varepsilon)\cdot\nu^0_{\alpha\beta}(t,x,x/\varepsilon) + \mathcal{O}(\varepsilon^2) \\ &= \varepsilon w^0_{\alpha\beta}(t,x,x/\varepsilon) + \mathcal{O}(\varepsilon^2) \quad \text{on } S^\varepsilon_{\alpha\beta}(t) \end{aligned} \tag{2}$$

For simplicity, we assume the *porosity* $\theta := 1 - |Y^0_s| > 0$ to be constant. The space- and time-dependent *saturation* is defined as $s(t,x) := |Y^0_1(t,x)|/\theta$. The ε-expansion of the concentrations is done analogously as in the well-known fixed-geometry case:

$$c^\varepsilon_1(t,x) = c^0_1\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon c^1_1\left(t,x,\frac{x}{\varepsilon}\right) + \cdots \quad \text{in } \Omega^\varepsilon_g(t) \tag{3}$$

$$c^\varepsilon_2(t,x) = c^0_2\left(t,x,\frac{x}{\varepsilon}\right) + \varepsilon c^1_2\left(t,x,\frac{x}{\varepsilon}\right) + \cdots \quad \text{in } \Omega^\varepsilon_1(t) \tag{4}$$

where the coefficient functions $c^i_1(t,x,y)$ and $c^i_2(t,x,y)$, $i \in \mathbb{N}$, are Y-periodic with respect to the variable y. For the nonlinear reaction rate, we assume:

$$\eta(c^\varepsilon_2) \approx \eta(c^0_2) + \mathcal{O}(\varepsilon) \tag{5}$$

Note that (5) is certainly true if g is linear. The asymptotic expansions (3) and (4) and the scaling relation (2) are plugged into (1) and the coefficients of different orders of ε are collected. Assuming that $|Y^0_g(t,x)| > 0$ for all t and x, we denote the *effective diffusivity* by:

$$D^*_1(t,x) := \frac{1}{|Y^0_g(t,x)|}\int\limits_{Y^0_g(t,x)} D_1[\delta_{ij} + \partial_{y_i}\varsigma_j]_{ij}\,\mathrm{d}y$$

For $j \in \{1,2\}$, the Y-periodic functions $\varsigma_j(t,x,\cdot)$ are solutions of the auxiliary problems:

$$\begin{aligned} &-\Delta\varsigma_j = 0 \quad \text{in } Y^0_g(t,x) \\ &\nabla_y\varsigma_j\cdot\nu^0 = -e_j\cdot\nu^0 \quad \text{on } \Gamma^0_{lg}(t,x)\cup\Gamma^0_{gs}(t,x) \end{aligned}$$

Omitting the upper index "0" at all quantities, the limit concentrations satisfy the following two-scale PDE system. The macroscopic equations are

$$\begin{aligned} &\partial_t\big((1-s)c_1\big) - \operatorname{div}\big((1-s)D^*_1\nabla c_1\big) \\ &\quad + \theta^{-1}H\int\limits_{\Gamma_{lg}} k_2(c_1-c_2) + (\delta_{j2}c_2 + \delta_{j3}H^{-1}c_1)w_{lg}\,\mathrm{d}\sigma_y = 0 \quad \text{in } \Omega \end{aligned} \tag{6a}$$

$$-D^*_1\nabla c_1\cdot\nu_\Gamma = b_1(c_1 - c^{\text{ext}}_1) \quad \text{on } \Gamma \tag{6b}$$

The local cell problem at each $x \in \Omega$ is given by:

$$\partial_t c_2 - \operatorname{div}_y(D_2\nabla_y c_2) + \eta(c_2) = 0 \quad \text{in } Y_1(t,x) \tag{6c}$$

$$-D_2\nabla_y c_2\cdot\nu_{lg} = k_2(c_2-c_1) - (\delta_{j2}-1)c_2 w_{lg} - \delta_{j3}H^{-1}c_1 w_{lg} \quad \text{on } \Gamma_{lg}(t,x) \tag{6d}$$

$$-D_2\nabla_y c_2\cdot\nu_{ls} - c_2 w_{ls} = 0 \quad \text{on } \Gamma_{ls}(t,x) \tag{6e}$$

The system (6) is a nonlinear parabolic system of partial differential equations with nonstandard coupling. We refer to it as **Problem ($\mathbf{T}_{\psi}^{\mathbf{nat}}$)**.

4. Weak formulation and analytical results

We derive a weak formulation of Problem ($\mathrm{T}_{\psi}^{\mathrm{nat}}$) in the time-dependent geometry. Let $S := [0, T]$ be some finite time interval. For a smooth test function $\varphi = \varphi(t, x)$ satisfying $\varphi|_{t=T} = 0$, we obtain from (6a), (6b):

$$\begin{aligned}
&-\int_S\int_\Omega (1-s)c_1\partial_t\varphi\,\mathrm{d}x\,\mathrm{d}t - \int_\Omega (1-s)c_1\varphi\,\mathrm{d}x\Big|_{t=0} + \int_S\int_\Omega (1-s)D_1^*\nabla c_1\nabla\varphi\,\mathrm{d}x\,\mathrm{d}t \\
&\quad + \int_S\int_\Gamma (1-s)b_1(c_1 - c_1^{\mathrm{ext}})\varphi\,\mathrm{d}\sigma_x\,\mathrm{d}t \\
&= \theta^{-1}H\int_S\int_\Omega\int_{\Gamma_{\mathrm{lg}}(t,x)} \big[k_2(c_2-c_1) - (\delta_{j2}c_2 + \delta_{j3}H^{-1}c_1)w_{\mathrm{lg}}\big]\varphi\,\mathrm{d}\sigma_y\,\mathrm{d}x\,\mathrm{d}t
\end{aligned} \tag{7}$$

The local cell problems (6c)–(6e) are multiplied by a smooth test function $\Phi = \Phi(t, x, y)$ depending on the fast variable $y \in Y_1$ and satisfying $\Phi|_{t=T} = 0$. Integration over Y_1, Ω and S gives:

$$\begin{aligned}
&-\int_S\int_\Omega\int_{Y_1(t,x)} c_2\partial_t\Phi\,\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}t - \int_\Omega\int_{Y_1(t,x)} c_2\Phi\,\mathrm{d}y\,\mathrm{d}x\Big|_{t=0} + \int_S\int_\Omega\int_{Y_1(t,x)} D_2\nabla_y c_2\nabla_y\Phi\,\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}t \\
&\quad + \int_S\int_\Omega\int_{\Gamma_{\mathrm{lg}}(t,x)} k_2(c_2-c_1) - (\delta_{j2}c_2 + \delta_{j3}H^{-1}c_1)w_{\mathrm{lg}}\,\Phi\,\mathrm{d}\sigma_y\,\mathrm{d}x\,\mathrm{d}t + \int_S\int_\Omega\int_{Y_1(t,x)} \eta(c_2)\Phi\,\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}t = 0
\end{aligned} \tag{8}$$

Since the geometry varies with time, the above weak formulation is not directly accessible to prove existence of solutions, for instance, by the method of a-priori estimates. However, this technique becomes applicable after transforming (8) to the reference geometry introduced above, provided that the transformation ψ and the velocity $\partial_t\psi$ admit first derivatives in z. It turns out that certain restrictions on the magnitude of the interfacial velocity w_{lg} are needed – depending on the interfacial condition type $j \in \{2, 3, 4\}$ – in order to guarantee pointwise bounds for the concentrations that are uniform in time. We state the main result of this analysis. For the proof and further details, we refer to [14] (Prop. 4.5.1 and Thm. 4.5.2) and forthcoming publications.

Theorem 4.1. *Assume that the interfacial velocity satisfies*:

$$w_{\mathrm{lg}} \begin{cases} \leqslant k_2 & \text{if } j = 2 \\ > -\min\{H, 1\}k_2 & \text{if } j = 3 \\ \geqslant -k_2 & \text{if } j = 4 \end{cases}$$

Then the Problem ($\mathrm{T}_{\psi}^{\mathrm{nat}}$) *possesses a unique weak solution in the sense of* (7) *and* (8). *The concentrations are uniformly bounded and there exist constants* $C_1, C_2 > 0$ *such that*:

$$\begin{aligned}
&\max_{0\leqslant t\leqslant T}\left(\int_\Omega |c_1|^2\,\mathrm{d}x + \int_\Omega\int_{Y_1(t,x)} |c_2|^2\,\mathrm{d}y\,\mathrm{d}x\right) + \int_S\left(\int_\Omega |\nabla c_1|^2\,\mathrm{d}x + \int_\Omega\int_{Y_1(t,x)} |\nabla_y c_2|^2\,\mathrm{d}y\,\mathrm{d}x\right)\mathrm{d}t \\
&\quad \leqslant C_1\left(|c_1|^2\,\mathrm{d}x + \int_\Omega\int_{Y_1(t,x)} |c_2|^2\,\mathrm{d}y\,\mathrm{d}x\right)\Big|_{t=0} + C_2\int_S |c_1^{\mathrm{ext}}|^2\,\mathrm{d}t
\end{aligned}$$

5. Reaction-driven evolution of the geometry

How can we model a phase evolution that is caused by the chemical reaction itself? The two-scale model (6) has to be complemented by an explicit evolution law for the transformation ψ. We suggest such a law for the case where

the liquid phase evolves due to production of water by the reaction. The model is similar as the one derived in [9] for evolving solid phase but includes a phase transition at the interfaces (namely, evaporation of water). The model is restricted to situations where the liquid phase remains disconnected from cell to cell.

Assumption B. The transformation ψ of the local cells can be parametrised by the saturation parameter s by means of a known mapping $\psi = \Psi(s)$.

More precisely, we assume there exist suitable values $0 < s_{\min} < s_{\max} < 1$ such that to each value $s \in [s_{\min}, s_{\max}]$ there corresponds a unique transformation $\psi = \Psi(s)$. We can therefore simply write $Y_1(s)$, $\Gamma_{\mathrm{lg}}(s)$, etc. The averaged mass balance of liquid water within one local cell can be formulated as an ordinary differential equation for s,

$$\partial_t s = \int_{Y_1(s)} A_3 \eta(c_2)\,\mathrm{d}y + \int_{\Gamma_{\mathrm{lg}}(s)} k_3\big(f(s_{\mathrm{eq}}) - f(s)\big)\,\mathrm{d}\sigma_y \tag{9}$$

where $A_3 > 0$ is a constant, s_{eq} is the equilibrium saturation and f describes the kinetics of evaporation at the gaseous–liquid interfaces. Eqs. (7), (8) together with (9) yield a closed system for determining c_1, c_2 and s, which is highly nonlinear. We refer to it as **Problem ($\mathbf{T_\Psi}$)**. By analogous transformation to reference coordinates, the following result can be established under slightly more smoothness assumptions.

Theorem 5.1. *If $\eta(c) \leqslant M_\eta$, then there exists constants $A_3^* = A_3^*(M_\eta) > 0$ and $k_2^* = k_2^*(M_\eta) > 0$ such that if $A_3 < A_3^*$ and $k_2 > k_2^*$, then the Problem* (T_Ψ) *possesses a unique solution.*

The proof relies on a fixed-point principle and is given in [14] (Thms. 5.3.9 and 5.4.3).

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