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Preprint 2012-09 Juni 2012

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A TWO-SCALE MODEL OF TWO-PHASE FLOW IN POROUS MEDIA RANGING FROM PORESPACE TO THE MACRO SCALE

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Abstract. We will derive two-scale models for two-phase flow in porous media, with the microscale given by the porescale. The resulting system will account for balance of mass, momentum and energy. To this aim, we will combine a generalization of Rajagopal's and Srinivasa's assumption of maximum rate of entropy production [39, 20, 21] with formal asymptotic expansion. The microscopic model will be based on phase fields, in particular to the full Cahn-Hilliard-Navier-Stokes-Fourier model derived in [23] with the boundary conditions from [20]. Using a generalized notion of characteristic functions, we will show that the solutions to the two-scale model macroscopically behave like classical solutions to a system of porous media flow equations. Relative permeabilities and capillary pressure relations are outcomes of the theory and exist only for special cases. Therefore, the two-scale model can be considered as a true generalization of classical models providing more information on the microscale thereby making the introduction of hysteresis superfluous.

1. Introduction

Flow in porous media is an old topic dating back to the pioneering publication by Darcy [10] who studied single phase flow in soil concluding that the velocity $\boldsymbol{v}$ depends on pressure p and gravitational potential $\boldsymbol{g}$ via

$$\boldsymbol{v} = A\,(\boldsymbol{g} - \nabla p) \tag{1.1}$$

where A is the permeability tensor. This relation has been investigated for a long time and has even mathematically been proven correct using homogenization techniques [2, 3, 4, 27, 35, 43].

However, problems arise at the moment the simple case of single phase flow is replaced by flows of at least two immiscible fluids, the root causes of these problems being *capillarity effects*: At the microscopic boundaries between the constituents, in particular at the contact lines on the solid's surfaces, capillary forces become important as they act on the small menisci. These forces strongly influence the evolution of microscopic geometry, which in turn has major impact on the soil's permeability for both fluids.

Capillary effects are usually taken into account by the following system of equations:

$$\begin{aligned} \partial_t\,(\varrho_a\theta_a) + \operatorname{div}\,(\varrho_a\theta_a\boldsymbol{v}_a) &= 0\,,\\ \partial_t\,(\varrho_w\theta_w) + \operatorname{div}\,(\varrho_w\theta_w\boldsymbol{v}_w) &= 0\,,\\ \theta_a + \theta_w = \Phi < 1\,, \end{aligned} \tag{1.2}$$

where Φ is the porosity (i.e. the volume fraction of the pore space) and θ_a and θ_w are the volume fractions of air and water and ϱ_a and ϱ_w the densities, respectively. In many applications, it is assumed that $\varrho_a = const$ and $\varrho_w = const$. In line with (1.1), the constitutive equations for $\boldsymbol{v}_a$ and $\boldsymbol{v}_w$ are assumed to be given through:

$$\begin{aligned} \boldsymbol{v}_w &= K_w(\dots)\,(\varrho_w\boldsymbol{g} - \nabla p_w)\ ,\\ \boldsymbol{v}_a &= K_a(\dots)\,(\varrho_a\boldsymbol{g} - \nabla p_a)\ , \end{aligned} \tag{1.3}$$

Date: 15.02.2012.

where p_a and p_w are the pressures in the air and water phase. The permeability tensors $K_{w/a}$ depend on several quantities such as porosity, microscopic geometry, $\theta_{w/a}$, $\varrho_{w/a}$ and others, where in most simple models, dependence of $K_{w/a}$ is restricted to θ_w or related quantities. For an overview over different models, refer to [26, 31, 42].

In order to complete the system, it is usually complemented with a constitutive relation between p_a and p_w of the form

$$p_w - p_a = p_c(\theta_w, \dots)\,, \tag{1.4}$$

where p_c is the so called *capillary pressure*. In case the air phase is connected with the atmosphere, it is commonly assumed that p_a equals the atmospheric pressure p_{atm}: $p_a = p_{atm}$. This assumption leads to Richards' equation, with air transport being neglected (as the mass of air is given by θ_w and p_{atm}) and the velocity of water is given through

$$\boldsymbol{v}_w = K_w(\dots)\left(\varrho_w \boldsymbol{g} - \nabla p_c(\theta_w)\right)\,.$$

Often, above models are incapable to describe real world phenomena, as long as they are based on a deterministic relation (1.4) and deterministic dependencies for $K_a(\theta_a)$ and $K_w(\theta_w)$. In particular, the last two assumptions for capillary pressure and permeabilities have been proven insufficient in many publications, refer to [17, 24, 28, 29, 30, 36, 37] and references therein.

In particular, it turns out that K_a and K_w are not only depending on θ_w but they are sensitive to the history of the system, as macroscopic permeability is not only due to water content, but also to microscopic distribution of phases, i.e. the microscopic geometry with its distribution of interfaces between water and air, of contact lines and contact angles.

The problem has been known for a long time and scientists tried to solve it introducing hysteresis operators. In particular the Preisach operator proved to be successful [13]. An overview over many classical models can be found in standard text books (for example [26, 31, 41, 42]) and in the large literature on the subject.

A mathematical introduction to hysteresis can be found in the book by Visintin [47]. Formally, Visintin characterizes Hysteresis as a "rate independent memory effect": the current state and development of a system depends on its history, in particular on all former states but not on the speed at which these states have been passed through. This applies for example to the "classically" used hysteresis models in porous media flow, such as the Preisach model [13]. Accordingly, measurements for drainage and imbibition curves are usually performed by measuring a series of steady states and in the resulting models, it is assumed that the relation $p_c(\theta)$ is independent on the speed of drainage and imbibition. Indeed, this approach was successful to some extend [13].

However, such macroscopic hysteretic behavior can be expected if and only if the macroscopic parameters like saturation and capillary pressure change slowly compared to the relaxation time on the micro scale. Thus, the faster macroscopic drainage or imbibition progress, the less reliable are the hysteretic models. In such cases, different approaches for the modeling of these memory effects are needed. Remark that already Hassanizadeh and Gray [18] showed that this does not hold in general and pointed out the limits of hysteresis approaches.

All these reflections point out that the usage of hysteresis operators or any macroscopic memory effect, reflects a lack of knowledge about "hidden" parameters, namely the microscopic distribution of the two phases, in particular the distribution of interfaces and contact lines on microscopic grain boundaries.

The approach and the results of this paper differ significantly from the usual approaches: The resulting system of equations will be defined on two scales and describe at the same time the macroscopic and the microscopic evolution of the system. Thus, the equations contain much more information about the system than in previous approaches. We will see further, that the resulting model is a true generalization of (1.2) and (1.3) as averaging the solution of the two-scale model yields macroscopic quantities that evolve according to equations of the form (1.2) and (1.3).

This will be achieved, combining the theory from recent papers by Heida, Málek and Rajagopal [23] and Heida [20] with formal asymptotic expansion. Note that the results from [20, 23] are obtained using a method first introduced by Rajagopal and Srinivasa [39] and generalized to boundary conditions in [20]. Shortly speaking, the paper is about homogenization of phase field models. We will work with a phase field model with the order parameter given in terms of concentrations but remark that generalization to more constituents, or to the description in terms of partial densities is obvious with respect to [23, 20][1]. The two constituents will be called water and air, for simplicity.

Note that the reasons for the choice of phase field models are threefold: In contrast with sharp interface models, phase field models allow for topological transitions in the geometry, an important effect in porous media flow. Also note that these are physical models, based on an early observation by Van der Waals [45, 46], and are not to be mixed up with the heuristic levelset approach. Third, in case of small pores, the effects due to the diffusive structure of the interface observed by Van der Waals may no longer be negligible.

Of course, the validity of the resulting two-scale equations strongly depends on the validity of the constitutive equations for the energy in bulk and on the microscopic boundaries. In particular, the constitutive equations for the energy which are used below are assumed to be valid for moderate temperatures as well as under moderate pressures. Also they only hold for a pore size which is still large compared to the transition zone. For example, if the transition zone is of order $10nm$, the pores should be of a size of at least $1\mu m$. For simplicity, we make the additional assumption that the two phases and the soil matrix share a common temperature field, i.e. that there are no temperature jumps on the microscopic boundaries. Finally, note that the soil matrix is assumed to be rigid. In particular, this implies that the medium under consideration is not deformable, which excludes effects like swelling.

To the authors knowledge, this is the very first attempt to derive such two-scale models for multiphase flow starting from the porescale using formal asymptotic expansion methods. A former attempt using REV-averaging can be found in in a recent paper by Papatzacos [38], but his approach and results differ significantly: REV averaging the way it was used in [38], is not suited to macroscopically resolve processes happening on a scale smaller than the poresize. Therefore, Papatzacos is not able to resolve the transition zone as phase interface inside the pore but he is restricted to the case when the transition zone is, in some sense, large compared to the pore diameter. Therefore he obtains a macroscopic Cahn-Hilliard system while we aim to recover macroscopic convective mass transport with Darcy-like constitutive equations for the velocity fields.

Concerning simulations, we mention a similar idea developed first by Gray and Hassanizadeh [14, 15, 16] who already stated that microscopic distribution of surfaces and contact lines is crucial for macroscopic behavior of the flow. This idea was further developed by Hassanizadeh and other coworkers like Celia, Dahle, Joekar-Niasar, Niessner, Norbotten and others [17, 28, 29, 30, 36, 37], who performed numerical calculations on a periodic structure of cells and channels in order to get macroscopic permeability depending on microscopic geometry and variation of geometry.

Hilfer [24, 25], initially also considering the microscopic distribution of interfaces as the main cause of macroscopic memory effects, recently started a new approach in terms of volume fractions, ending up with rate dependent pressure/saturation relations. Like for the present approach, he states that relative permeabilities as well as capillary pressure should be an outcome of theory and not an input.

Hassanizadeh and Gray as well as Hassanizadeh et.al. and Hilfer agree that capillary pressure is not a static variable. Also they claim that a hysteretic dependence on saturation is not enough to capture all dynamic phenomena. Rather they state that the capillary pressure is a dynamic variable that depends on saturation as well as on the microscopic distribution of phase interfaces (menisci)

[1]Such a generalization can be found in Heida [19] for permafrost soil, a system with the constituents air, water, ice and vapor.

and contact lines. Once these phenomena are incorporated to the models, hysteresis is no longer in need.

Finally, Hassanizadeh and Gray [18] state that capillary pressure can hardly be obtained from microscopic point of view, as the pressure drop across the water/air interface strongly depends on geometry. This is the reason why this article will abstain from providing explicit formulas for the capillary pressure difference except for a small outlook in section 12 in case of Richards equation. This topic is left for future investigations and for numerical experiments. Former investigations from the theoretical point of view, also including averaging calculations, can be found in [36, 37] among which the closest to the present approach is by Norbotten et. al. [37].

The structure of the article is as follows: In section 2 we will introduce some important standard notations that will be frequently used throughout the article. In 3 we will introduce the formal asymptotic expansion method for the derivation of two-scale models and exemplarily derive Darcy's law, also for the purpose of providing better understanding of sections 8-11. After that, we will introduce abstract equations of continuum mechanics (section 4), describe how the abstract equations can be non-dimensionalized (section 5) and how thermodynamically consistent constitutive equations can be derived using Rajagopal's and Srinivasa's assumption of maximum rate of entropy production within the generalized framework by Heida [19, 20] and Heida, Málek and Rajagopal [21] (section 6). Then, we will finally derive the microscopic model in the porespace 7 and the two-scale model 8.

The coupled two-scale system in itself already is a complete model for two-phase flow in porous media. Nevertheless, we also provide calculations to estimate the effective macroscopic behavior of the solutions and yielding that solutions to the resulting two-scale equations show the expected (and usually observed) macroscopic behavior in sections 10-11.

The resulting macroscopic balance of energy will consist of Fourier's law with convection (section 10). The balances of mass for water and air will be given through convection equations (section 10). The most problematic part is the derivation of constitutive equations for the macroscopic velocities of water and air.

It will be shown, that once a solution to the two-scale equation is found, it is possible to split up the balance of momentum into two separate equations for the velocity fields of air and water (section 11). The basic idea of this splitting is, that the physics in the bulk differs significantly from the physics close to the transition zone which will also be reflected in the new system. The separated equations will be highly coupled through the transition zone and will only decouple in case of stationary geometry.

Note that the equations point out that macroscopic equations like the Richard's equation cannot be obtained but in very special cases. Nevertheless, we will shortly discuss this topic in section 12.

2. Preliminaries

2.1. **Geometric setting.** Throughout this article, we will consider a bounded and open domain $\boldsymbol{Q} \subset \mathbb{R}^3$. Furthermore, consider $\boldsymbol{Y} := [0,1[^3$, with $\boldsymbol{Y} = \boldsymbol{Y}_1 \cup \boldsymbol{Y}_2 \cup \Gamma$ such that $\Gamma := \partial\boldsymbol{Y}_1 \cap \partial\boldsymbol{Y}_2 \cap \boldsymbol{Y}$. We expand $\boldsymbol{Y}$, $\boldsymbol{Y}_1$, $\boldsymbol{Y}_2$ and Γ periodically to $\mathbb{R}^3$ assuming that the periodizations of $\boldsymbol{Y}_1$ and $\boldsymbol{Y}_2$ are both simply connected and open in $\mathbb{R}^3$ and $\Gamma := \partial\boldsymbol{Y}_1 \cap \partial\boldsymbol{Y}_2$. We multiply the resulting structures by ε to obtain $\boldsymbol{Y}_1^\varepsilon = \varepsilon\boldsymbol{Y}_1$, $\boldsymbol{Y}_2^\varepsilon = \varepsilon\boldsymbol{Y}_2$ and $\Gamma^\varepsilon = \varepsilon\Gamma$. Finally, we define the following subsets of $\boldsymbol{Q}$: $\boldsymbol{Q}_1^\varepsilon := \boldsymbol{Q} \cap \boldsymbol{Y}_1^\varepsilon$, the pore space, and $\boldsymbol{Q}_2^\varepsilon := \boldsymbol{Q} \cap \boldsymbol{Y}_2^\varepsilon$, the solid matrix. Wherever it will not provoke any confusion, we equally denote $\Gamma^\varepsilon := \partial\boldsymbol{Q}_1^\varepsilon \cap \boldsymbol{Q}$. The definitions are illustrated in figure 2.1. The outer normal vector of $\boldsymbol{Y}_1$ on Γ will be called $\boldsymbol{n}_\Gamma$ and the outer normal vector of $\boldsymbol{Q}_1^\varepsilon$ on Γ^ε is denoted as $\boldsymbol{n}_{\Gamma^\varepsilon}$.

One should be very careful in not mixing up the periodic cell $\boldsymbol{Y}$ with the notion of a so called "Representative Elementary Volume" (REV) that is used in applied sciences such as soil physics. The REV is a volume that is big compared to micro structures but small compared to the macroscopic scale. Therefore, a single cell $\varepsilon\boldsymbol{Y}$ is not suitable, neither $\boldsymbol{Y}$. For example, Joekar-Niasar et. al.

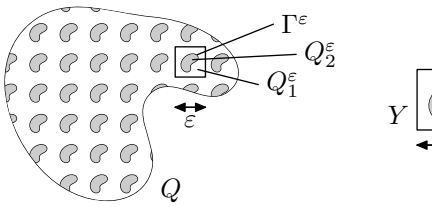

FIGURE 2.1. Sketch of geometrical setting and notation.

[28] found in their simulations, that an REV is at least of the size $40 \times 40 \times 40$ periodic cells. An introduction to the REV-averaging method can be found for example in the book by Dormieux, Kondo and Ulm [11]; it should not be mixed up with the present method of formal asymptotic expansion.

However, given such $\boldsymbol{Q}$, $\boldsymbol{Y}_1^\varepsilon$ and $\boldsymbol{Y}_2^\varepsilon$, we identify εL_0 as the parameter describing the typical size of a pore, where w.l.o.g. $L_0 = 1$ is the macroscopic length scale. With respect to application, ε is depending on the physical size of the pores and the complexity of the geometry, which is represented by $\boldsymbol{Y}$, $\boldsymbol{Y}_1$ and $\boldsymbol{Y}_2$. In any case, from the physical point of view, ε is a fixed parameter. In order to derive two-scale models, it is important to seek for a suitable non dimensionalization of the physical equations. This is topic of section 5.

2.2. **Differential Operators on the Boundary.** On Γ, let $\boldsymbol{n}_\Gamma$ be the normal vector field and for each arbitrary vector field $\boldsymbol{a} : \Gamma \to \mathbb{R}^3$, we define the normal part a_n and the tangential part $\boldsymbol{a}_\tau$ via

$$a_n := \boldsymbol{a} \cdot \boldsymbol{n}_\Gamma, \qquad \boldsymbol{a}_\tau := \boldsymbol{a} - a_n \boldsymbol{n}_\Gamma \,.$$

We define the normal derivative of a scalar quantity a through

$$\partial_n a := \nabla a \cdot \boldsymbol{n}_\Gamma$$

and the tangential gradient ∇_τ for such scalars through

$$\nabla_\tau a := (\nabla a)_\tau = \nabla a - \boldsymbol{n}_\Gamma \partial_n a \,.$$

For any vector field $\boldsymbol{f}_\tau$ tangential to Γ, we define the divergence

$$\mathrm{div}_\tau \boldsymbol{f}_\tau := \mathrm{tr} \nabla_\tau \boldsymbol{f}_\tau \,.$$

and we find:

$$\mathrm{div}\, \boldsymbol{f} = \mathrm{div}_\tau \boldsymbol{f} + \partial_n(\boldsymbol{f}_n) \,.$$

The mean curvature of Γ is defined as

$$\kappa_\Gamma := \mathrm{trace}\,(\nabla_\tau \boldsymbol{n}_\Gamma)$$

and we find the following important result:

Lemma 1. *(See for example* [6]*) For any $f \in C^1(\Gamma)$ holds*

$$\int_\Gamma \nabla_\tau f = \int_\Gamma f \kappa_\Gamma \boldsymbol{n}_\Gamma + \int_{\partial\Gamma} f \boldsymbol{\nu}$$

where $\boldsymbol{\nu}^* := (\boldsymbol{n}_{\partial \boldsymbol{Q}})_\tau$ and $\boldsymbol{\nu} = |\boldsymbol{\nu}^*|^{-1} \boldsymbol{\nu}^*$ is the unit vector tangent to Γ and normal to $\partial\Gamma$. Furthermore, for any tangentially differentiable field $\boldsymbol{q}$ holds

$$\int_\Gamma div_\tau \boldsymbol{q} = \int_\Gamma \kappa_\Gamma \boldsymbol{q} \cdot \boldsymbol{n}_\Gamma + \int_{\partial\Gamma} \boldsymbol{q} \cdot \boldsymbol{\nu}$$

Note that the Laplace-Beltrami operator on Γ is then defined by

$$\Delta_{\tau\tau} f = \mathrm{div}_\tau \nabla_\tau f$$

and Lemma 1 yields for any continuously differentiable and tangential vector field $\boldsymbol{f} = \boldsymbol{f}_\tau$ on Γ

$$\int_\Gamma \mathrm{div}_\tau \boldsymbol{f} = 0\,. \tag{2.1}$$

3. Asymptotic Expansion and Darcy's Law

Asymptotic expansion, as it will be applied below, is not a mathematically rigorous but only formal modeling tool. Given a microscopic geometry on $\boldsymbol{Q}$ by $\boldsymbol{Y}_1^\varepsilon$, $\boldsymbol{Y}_2^\varepsilon$ and Γ^ε, it starts from a set of (partial) differential equations, the *microscopic problem*, which depends on the geometry and on ε. It is the aim of homogenization to investigate the behavior of solutions to the microscopic problem as $\varepsilon \to 0$ and to identify approximating macroscopic or two-scale problems. In particular, the approximating problem often is not only defined on $\boldsymbol{Q}$ but on $\boldsymbol{Q} \times \boldsymbol{Y}$ although there are special cases where a reduction to a problem on $\boldsymbol{Q}$ is possible. This will be the case for the derivation of Darcy's law below.

Note that there is big amount of literature on homogenization. Below, we will deal with homogenization of Cahn-Hilliard-Navier-Stokes-Fourier systems, thus we get in touch with Stokes and Laplace operators. For former results on the homogenization of Navier-Stokes and Stokes flow, refer to works by Allaire [1, 2, 3], Ene and Saint Jean Paulin [12], Marušić-Paloka [32], Mikelić [33, 35], Sandrakov [44] and of course the pioneering work by Tartar in the appendix of [43]. For the homogenization of diffusion and diffusion with nonlinear boundary conditions, the reader is referred to Amaziane, Goncharenko and Pankratov [5], Conca, Diaz and Timofte [9], Conca, Diaz, Liñan and Timofte [8], Heida [19], Hornung [27], Mikelić and Primicerio [34] and the references therein.

Considering any ε-dependent unknown u^ε, the basic idea of asymptotic expansion is an ansatz

$$u^\varepsilon = \sum_{i=0}^{\infty} \varepsilon^i u_i^\varepsilon\,, \tag{3.1}$$

where the functions u_i^ε have to be specified. Since the domain $\boldsymbol{Q} = \boldsymbol{Q}_1^\varepsilon \cup \boldsymbol{Q}_2^\varepsilon \cup \Gamma^\varepsilon$ is characterized by, $\boldsymbol{Q}$ and $\boldsymbol{Y} = \boldsymbol{Y}_1 \cup \boldsymbol{Y}_2 \cup \Gamma$ and ε, it seems reasonable to assume that $u_i : [0,T] \times \boldsymbol{Q} \times \mathbb{R}^3 \to \mathbb{R}^k$ with u_i being $\boldsymbol{Y}$-periodic in the third variable. In particular

$$\begin{aligned} u_i : [0,T] \times \boldsymbol{Q} \times \boldsymbol{Y} &\to \mathbb{R}^k \\ (t,x,y) &\mapsto u_i(t,x,y)\,, \end{aligned}$$

with

$$u_i^\varepsilon(t,\cdot) := u_i\left(t,\cdot,\frac{\cdot}{\varepsilon}\right)$$

and (3.1) becomes

$$u^\varepsilon(t,\cdot) = \sum_{i=0}^{\infty} \varepsilon^i u_i(t,\cdot,\frac{\cdot}{\varepsilon}). \tag{3.2}$$

Additionally, the following relations for the gradient and the divergence operators hold:

$$\nabla = \nabla_x + \frac{1}{\varepsilon}\nabla_y, \quad \mathrm{div} = \mathrm{div}_x + \frac{1}{\varepsilon}\mathrm{div}_y\,. \tag{3.3}$$

Inserting (3.3) together with (3.2) into the particular partial differential equation, separating powers of ε, we obtain effective equations for the approximate behavior of $u^\varepsilon(t,\cdot) \approx u_0(t,\cdot)$. We will start by considering homogenization of the Stokes equations with the scaling introduced by Allaire [4] (see also [27, chapter 3]).

3.1. **Homogenization of the incompressible Stokes equation: Dynamic case.** We start with the incompressible Stokes fluid. Incompressibility implies that the pressure p^ε is an unknown, density is constant and the velocity $\boldsymbol{v}^\varepsilon$ has to fulfill the incompressibility condition (3.4b):

$$\partial_t \boldsymbol{v}^\varepsilon - \varepsilon^2 \mathrm{div}\,(\mu \nabla \boldsymbol{v}^\varepsilon) + \nabla p^\varepsilon = \boldsymbol{g}^\varepsilon \quad \text{on } \boldsymbol{Q}_1^\varepsilon \tag{3.4a}$$

$$\mathrm{div}\,\boldsymbol{v}^\varepsilon = 0 \quad \text{on } \boldsymbol{Q}_1^\varepsilon \tag{3.4b}$$

$$\boldsymbol{v}^\varepsilon = 0 \quad \text{on } \partial \boldsymbol{Q}_1^\varepsilon \tag{3.4c}$$

$$\boldsymbol{v}^\varepsilon = 0 \quad \text{on } \boldsymbol{Q}_2^\varepsilon \tag{3.4d}$$

With an additional initial condition on $(0,T] \times \boldsymbol{Q}$ of the form

$$\boldsymbol{v}^\varepsilon(0,\cdot) = \tilde{\boldsymbol{v}}_0(\cdot, \frac{\cdot}{\varepsilon})\,.$$

We assume that $\boldsymbol{g}^\varepsilon(x) = \boldsymbol{g}(x)$ and there is a family of functions

$$\begin{aligned} \boldsymbol{v}_i : [0,T] \times \boldsymbol{Q} \times Y &\to \mathbb{R}^3 \qquad 0 \le i < \infty \\ (t,x,y) &\mapsto \boldsymbol{v}_i(t,x,y) \\ p_i : [0,T] \times \boldsymbol{Q} \times Y &\to \mathbb{R}^3 \qquad 0 \le i < \infty \\ (t,x,y) &\mapsto p_i(t,x,y) \end{aligned}$$

such that the solution $\boldsymbol{v}^\varepsilon$ and p^ε can be described by

$$\boldsymbol{v}^\varepsilon(t,\cdot) = \sum_{i=0}^{\infty} \varepsilon^i \boldsymbol{v}_i(t,\cdot,\frac{\cdot}{\varepsilon}) \tag{3.5a}$$

$$p^\varepsilon(t,\cdot) = \sum_{i=0}^{\infty} \varepsilon^i p_i(t,\cdot,\frac{\cdot}{\varepsilon}) \tag{3.5b}$$

where the functions $\boldsymbol{v}_i$ and p_i are periodic in Y. The first coordinate reflects the macroscopic behavior of the solution, while the second coordinate reflects microscopic variations due to presence of microscopic geometry. The basic Idea is to insert (3.5) together with (3.3) into (3.4a) and separate the terms by powers of ε such that equations (3.4) take the form

$$\varepsilon^{-1}(\dots) + \varepsilon^0(\dots) + \mathcal{O}(\varepsilon) = 0\,.$$

In particular, the result reads up to order 0:

$$\varepsilon^{-1}\nabla_y p_0 + \varepsilon^0 \left(\partial_t \boldsymbol{v}_0 - \mathrm{div}_y\,(\mu \nabla_y \boldsymbol{v}_0) + \nabla_x p_0 + \nabla_y p_1 - \boldsymbol{g}\right) + \mathcal{O}(\varepsilon) = 0 \tag{3.6a}$$

$$\varepsilon^{-1}\mathrm{div}_y\,\boldsymbol{v}_0 + \mathrm{div}_x\,\boldsymbol{v}_0 + \mathrm{div}_y\,\boldsymbol{v}_1 + \mathcal{O}(\varepsilon) = 0 \tag{3.6b}$$

$$\sum_i \varepsilon^i \boldsymbol{v}_i(t,x,\cdot) = 0 \quad \text{on } \partial Y_1, \quad \sum_i \varepsilon^i \boldsymbol{v}_i(t,\cdot,y) = 0 \quad \text{on } \partial \boldsymbol{Q} \tag{3.6c}$$

For each power of ε, a new set of equations is obtained, which has to hold independently on ε.

Order -1 of (3.6a) yields $\nabla_y p_0 = 0$. For order 0 of that same equation, the resulting system with order -1 in (3.6b) reads

$$\begin{aligned} \partial_t \boldsymbol{v}_0 - \mathrm{div}_y\,(\mu \nabla_y \boldsymbol{v}_0) + \nabla_x p_0 + \nabla_y p_1 &= \boldsymbol{g} \\ \mathrm{div}_x\,\boldsymbol{v}_0 &= 0 \\ \mathrm{div}_y\,\boldsymbol{v}_0 &= 0\,. \end{aligned}$$

This is a complete two-scale model for $\boldsymbol{v}_0$ and represents as such a solution to the homogenization problem. Thus, we can consider either

$$\boldsymbol{v}_0(\cdot, \frac{\cdot}{\varepsilon}) \qquad \text{or} \qquad \boldsymbol{v}_{eff} := \int_{\boldsymbol{Y}} \boldsymbol{v}_0(\cdot, y)\, dy$$

as an approximation of $\boldsymbol{v}^\varepsilon(\cdot)$, where the quality of this approximation is measured in terms of

$$\left\| \boldsymbol{v}^\varepsilon(\cdot) - \boldsymbol{v}_0(\cdot, \frac{\cdot}{\varepsilon}) \right\|_{L^2(\boldsymbol{Q})} \qquad \text{or} \qquad \left\| \boldsymbol{v}^\varepsilon(\cdot) - \boldsymbol{v}_{eff}(\cdot) \right\|_{L^2(\boldsymbol{Q})} .$$

However, in laboratory experiments and in nature, we are interested the macroscopic behavior of $\boldsymbol{v}_{eff}$. To obtain a macroscopic description for the evolution of $\boldsymbol{v}_{eff}$, we consider $\boldsymbol{u}_i$ solutions to

$$\begin{aligned} \partial_t \boldsymbol{u}_i - \operatorname{div}_y (\mu \nabla_y \boldsymbol{u}_i) + \nabla_y \Pi_i &= \boldsymbol{e}_i \quad \text{on }]0,T] \times \boldsymbol{Y}_1 \\ \operatorname{div}_y \boldsymbol{u}_i &= 0 \quad \text{on }]0,T] \times \boldsymbol{Y}_1 \\ \boldsymbol{u}_i(0,\cdot) &= \boldsymbol{0} \quad \text{on } \boldsymbol{Y}_1 \\ \boldsymbol{u}_i(\cdot,\cdot) &= \boldsymbol{0} \quad \text{on } [0,T] \times \partial \boldsymbol{Y}_1 \end{aligned}$$

where $\boldsymbol{e}_i$ is the i-th standard basis vector of $\mathbb{R}^3$. We furthermore introduce $\hat{\boldsymbol{v}}$ through

$$\hat{\boldsymbol{v}}(t,x,y) := \int_0^t \sum_i \left[\partial_t \left(\boldsymbol{g} - \nabla_x p_0\right)_i (s,x)\right] \boldsymbol{u}_i(t-s,x,y) ds\,.$$

Since

$$\begin{aligned} \partial_t \hat{\boldsymbol{v}}(t,x,y) = &\int_0^t \sum_i \left[\partial_t \left(\boldsymbol{g} - \nabla_x p_0\right)_i (s,x)\right] \partial_t \boldsymbol{u}_i(t-s,x,y) ds \\ &+ \sum_i \left[\partial_t \left(\boldsymbol{g} - \nabla_x p_0\right)_i (t,x)\right] \boldsymbol{u}_i(0,x,y)\,, \end{aligned}$$

we find due to the initial conditions on $\boldsymbol{u}_i$:

$$\partial_t \hat{\boldsymbol{v}} - \operatorname{div}_y\, (\mu \nabla_y \hat{\boldsymbol{v}}) = \boldsymbol{g} - \nabla p_0 - \nabla_y \int_0^t \sum_i \left[\partial_t \left(\boldsymbol{g} - \nabla_x p_0\right)_i (s,x)\right] \Pi_i ds\,,$$

and the velocity field can be split up into

$$\boldsymbol{v}_0 = \tilde{\boldsymbol{v}} + \hat{\boldsymbol{v}}$$

where

$$\begin{aligned} \partial_t \tilde{\boldsymbol{v}} - \operatorname{div}_y\, (\mu \nabla_y \tilde{\boldsymbol{v}}) + \nabla_y \boldsymbol{q}_1 &= \boldsymbol{0} \qquad \text{on } (0,t) \times \boldsymbol{Y}_1 \\ \operatorname{div}_y \tilde{\boldsymbol{v}} &= 0 \qquad \text{on } (0,t) \times \boldsymbol{Y}_1 \\ \tilde{\boldsymbol{v}} &= \boldsymbol{0} \qquad \text{on } (0,t) \times \Gamma \\ \tilde{\boldsymbol{v}}(0,\cdot) &= a(\cdot) \quad \text{on } \boldsymbol{Y}_1\,. \end{aligned}$$

Defining

$$A_{i,j} := \partial_t \int_{\boldsymbol{Y}_1} \boldsymbol{u}_i \cdot \boldsymbol{e}_j$$

one may check by partial integration, the initial conditions on $\boldsymbol{u}_i$ and the assumption $\left(\boldsymbol{g} - \nabla p\right)\Big|_{t=0} = 0$ that

$$\boldsymbol{v}_{eff} = \int_{\boldsymbol{Y}_1} \tilde{\boldsymbol{v}} + \int_0^t A(t-s) \left(\boldsymbol{g} - \nabla_x p_0\right)(s) ds\,,$$

where $\tilde{\boldsymbol{v}} \to \boldsymbol{0}$ pointwise as $t \to \infty$. For a rigorous proof of this homogenization result refer to Allaire [27, chapter 3].

3.2. **The Stationary Case.** For the stationary case in (3.4), i.e. $\partial_t \boldsymbol{v}^\varepsilon = 0$, we end up with [27]

$$\boldsymbol{v}_{eff} = \int_{\boldsymbol{Y}} \boldsymbol{v}_0 = A\left(\boldsymbol{g} - \nabla_x p_0\right)$$

where

$$A_{i,j} := \int_{\boldsymbol{Y}_1} \boldsymbol{u}_i \cdot \boldsymbol{e}_j$$

and $\boldsymbol{u}_i$ are solution to

$$\begin{aligned} -\mathrm{div}_y\left(\mu \nabla_y \boldsymbol{u}_i\right) + \nabla_y \Pi_i &= \boldsymbol{e}_i \quad \text{on } \boldsymbol{Y}_1 \\ \mathrm{div}_y\, \boldsymbol{u}_i &= 0 \quad \text{on } \boldsymbol{Y}_1 \\ \boldsymbol{u}_i(x,\cdot) &= \boldsymbol{0} \quad \text{on } \partial \boldsymbol{Y}_1\,. \end{aligned}$$

4. Continuum Mechanics

We follow the outline of previous works by Heida, Málek and Rajagopal [23, 22] on phase field models as well as [20], where the author introduced a new method to derive thermodynamically consistent boundary conditions for phase field models.

4.1. **The Porespace.** Thus, on $\boldsymbol{Q}_1^\varepsilon$, we assume the presence of a mixture consisting of two different (almost) immiscible species, which we call without loss of generality water and air, having partial densities ϱ_w and ϱ_a. Assuming mass conservation for both species and transported by partial velocities $\boldsymbol{v}_w$, $\boldsymbol{v}_a$ we obtain mass balance equations of the form

$$\partial_t \varrho_i + \mathrm{div}\,\left(\varrho_i \boldsymbol{v}_i\right) = 0 \qquad i \in \{a, w\}\,. \tag{4.1}$$

In particular, we exclude production of air and water and chemical reactions, for simplicity. The densities ϱ_a and ϱ_w add up to a total density ϱ of the mixture and the momenta of air and water add up to the total momentum $\varrho\boldsymbol{v}$, introducing by the same time the mean velocity $\boldsymbol{v}$ of the mixture through:

$$\varrho = \varrho_a + \varrho_w, \qquad \boldsymbol{v} := \frac{1}{\varrho}\left(\varrho_a \boldsymbol{v}_a + \varrho_w \boldsymbol{v}_w\right)\,.$$

Therefore, we can formulate the mixture's balance of mass as

$$\partial_t \varrho + \mathrm{div}\,\left(\varrho \boldsymbol{v}\right) = 0\,.$$

Defining the material derivative for scalars a and vectors $\boldsymbol{f}$ through

$$\dot{a} := \partial_t a + \boldsymbol{v}\cdot\nabla a, \qquad \dot{\boldsymbol{f}} := \partial_t \boldsymbol{f} + \left(\nabla \boldsymbol{f}\right)\boldsymbol{v} \tag{4.2}$$

we get with

$$c := \frac{\varrho_w}{\varrho}, \qquad \boldsymbol{j} := \left(\boldsymbol{v}_w - \boldsymbol{v}\right)\varrho_w$$

and $(4.1)_w$:

$$\varrho \dot{c} + \mathrm{div}\,\boldsymbol{j} = 0\,.$$

Following the approach by Heida, Málek and Rajagopal [23, 22], we are not interested in the balance of energy, momentum and angular momentum for each constituent but postulate that the mixture is sufficiently described by the balance of energy, momentum and angular momentum for the mixture as a whole. As pointed out in [23], this is useful if we are not interested in energy and momentum exchange between the several constituents.

Thus, introducing the Cauchy stress $\mathbb{T}$, the internal energy per mass u, the total energy per mass $E := \frac{1}{2}\left|\boldsymbol{v}^2\right| + u$, the diffusive heat flux $\boldsymbol{j}_E$, external energy supply s and external body force $\boldsymbol{g}$, we require the validity of the following set of equations:

$$\begin{aligned} \partial_t\left(\varrho\boldsymbol{v}\right) + \mathrm{div}\,\left(\varrho\boldsymbol{v}\otimes\boldsymbol{v}\right) - \mathrm{div}\,\mathbb{T} &= \boldsymbol{g} \qquad\qquad \mathbb{T} = \mathbb{T}^T \\ \partial_t\left(\varrho E\right) + \mathrm{div}\,\left(\varrho E \boldsymbol{v}\right) - \mathrm{div}\,\left(\mathbb{T}\boldsymbol{v} + \boldsymbol{j}_E\right) &= s\,. \end{aligned}$$

As pointed out in [23], introducing

$$\boldsymbol{h} := \mathbb{T}\boldsymbol{v} + \boldsymbol{j}_E$$

leads to the system

$$\begin{aligned} \dot{\varrho} + \varrho \operatorname{div} \boldsymbol{v} = 0 \quad \varrho\dot{\boldsymbol{v}} - \operatorname{div} \mathbb{T} = \boldsymbol{g} \quad \mathbb{T} = \mathbb{T}^T \\ \varrho\dot{c} + \operatorname{div} \boldsymbol{j} = 0 \quad \varrho\dot{E} - \operatorname{div} \boldsymbol{h} = s\,. \end{aligned} \tag{4.3}$$

While up to now, these equations do not account for any interaction between the two constituents water and air, note that such information will enter due to constitutive equations on $\mathbb{T}$, $\boldsymbol{j}$ and $\boldsymbol{h}$ which will be derived below.

4.2. **The Solid Matrix.** On $\boldsymbol{Q}_2^\varepsilon$, the solid Matrix, the velocity field is zero, the density is stationary and we do not consider any dynamics except for energy transport. Writing E_2 for the energy per volume in $\boldsymbol{Q}_2^\varepsilon$ and $\boldsymbol{h}_2$ for the diffusive energy flux, the balance of energy reads

$$\partial_t E_2 - \operatorname{div} \boldsymbol{h}_2 = 0\,, \tag{4.4}$$

as we assume no external (external of $\boldsymbol{Q}$) supply of energy to the solid matrix.

4.3. **The Microscopic Boundary.** Following [20], we assume the presence of a surface energy field E_Γ on Γ^ε and assume that it evolves due to

$$\partial_t E_\Gamma - \operatorname{div} \boldsymbol{h}_\Gamma = \overset{\oplus}{E} \tag{4.5}$$

where $\boldsymbol{h}_\Gamma$ is some surface energy flux and $\overset{\oplus}{E}$ is supply of energy from the bulk to Γ^ε. Note that E_Γ is not the trace of E or E_2 on Γ^ε. Indeed, E is measured in energy per mass, E_2 is measured in energy per volume and E_Γ in energy per area. However, due to $\boldsymbol{h}$, $\boldsymbol{h}_2$ and $\overset{\oplus}{E}$, there is an exchange of energy between $\boldsymbol{Q}_1^\varepsilon$, $\boldsymbol{Q}_2^\varepsilon$ and Γ^ε, as demonstrated in section 6.1.

As will be shown in section 7 we also have to account for an additional boundary condition for c which is of the form

$$\varrho\partial_t c + \varrho \boldsymbol{v}_\tau \cdot \nabla_\tau c = \overset{\oplus}{c}\,. \tag{4.6}$$

5. Non-Dimensionalization

The equations of balance for ϱ, c and E in system (4.3) can be brought to a form

$$\partial_t \phi + \operatorname{div}\,(\boldsymbol{v}\phi) + \operatorname{div} \boldsymbol{j}_\phi = 0\,, \qquad \phi \in \{\varrho, c, E\} \tag{5.1}$$

while the balance of momentum takes the form

$$\partial_t\,(\varrho\boldsymbol{v}) + \operatorname{div}\,(\varrho\boldsymbol{v} \otimes \boldsymbol{v}) - \operatorname{div} \mathbb{T} = \boldsymbol{g}\,. \tag{5.2}$$

We want to study the behavior of these equations with respect to the characteristic scales of the physical setting: We assume that the characteristic scale of space is given by L_0, the characteristic scale of time is given by t_0 and the characteristic scales of ϱ, c, E, $\boldsymbol{v}$, $\boldsymbol{j}_\phi$ and $\mathbb{T}$ by ϱ^*, c^*, E^*, v^*, j_ϕ^* and T^* respectively. (Note that these scales may depend on ε as they may depend on the ratio between macroscopic and microscopic length scales. Furthermore, note that v^*, j_ϕ^* and T^* are scalars!) The non dimensionalized quantities are indicated by an upper index ε, thus by ϕ^ε, $\boldsymbol{v}^\varepsilon$, $\mathbb{T}^\varepsilon$, $\boldsymbol{j}_\phi^\varepsilon$. We find

$$\phi = \phi^*\phi^\varepsilon, \quad \boldsymbol{v} = v^*\boldsymbol{v}^\varepsilon, \quad \mathbb{T} = T^*\mathbb{T}^\varepsilon, \quad \boldsymbol{j}_\phi = j_\phi^*\boldsymbol{j}_\phi^\varepsilon\,,$$

and insert these relations in (5.1) and (5.2), having in mind

$$\operatorname{div} = L_0^{-1}\operatorname{div}^*\,, \qquad \nabla = L_0^{-1}\nabla^*\,, \qquad \partial_t = t_0^{-1}\partial_t^*\,,$$

where div^*, ∇^* and ∂_t^* are derivatives with respect to $\frac{x}{L_0}$ and $\frac{t}{t_0}$. We find

$$\partial_t^* \phi^\varepsilon + \frac{t_0 v^*}{L_0} \mathrm{div}^* \left(\boldsymbol{v}^\varepsilon \phi^\varepsilon\right) + \frac{t_0 j_\phi^*}{L_0 \phi^*} \mathrm{div}^* \boldsymbol{j}_\phi^\varepsilon = 0\,, \qquad \phi \in \{\varrho, c, E\} \tag{5.3}$$

$$\partial_t^* \left(\varrho^\varepsilon \boldsymbol{v}^\varepsilon\right) + \frac{t_0 v^*}{L_0} \mathrm{div}^* \left(\varrho^\varepsilon \boldsymbol{v}^\varepsilon \otimes \boldsymbol{v}^\varepsilon\right) - \frac{t_0 T^*}{L_0 \varrho^* v^*} \mathrm{div}^* \mathbb{T} = \boldsymbol{g}\,. \tag{5.4}$$

It is one of the most crucial steps in homogenization to identify the correct scales of the factors

$$\frac{t_0 v^*}{L_0}\,, \qquad \frac{t_0 j_\phi^*}{L_0 \phi^*}\,, \qquad \text{and} \qquad \frac{t_0 T^*}{L_0 \varrho^* v^*}\,. \tag{5.5}$$

In classical approaches to homogenization, these scales are identified after the constitutive equations for $\boldsymbol{j}$, $\boldsymbol{h}$ and $\mathbb{T}$ in (4.3) have been provided from theory.

However, there is one problematic issue connected with this approach: Even if constitutive equations have been derived from thermodynamic principles, it is by no means clear that the non-dimensionalization and identification of ε yields thermodynamically consistent systems of equations for all ε. If the scaling of the equations would lead to a violation of the second law for small ε, the resulting homogenized equations would not be thermodynamically consistent and make the result doubtable.

Therefore, we will follow a different path: We will start by identifying the reasonable scales for (5.5). Then, we will directly derive non-dimensionalized constitutive equations for $\boldsymbol{j}^\varepsilon$, $\boldsymbol{h}^\varepsilon$ and $\mathbb{T}^\varepsilon$, using (5.3), (5.4) and the method of maximum rate of entropy production.

First note that the scaling in front of the convective term is the same for all quantities. We will assume that convection is small on the macro scale, i.e. that infiltration rates to the porous medium are low. Thus, it is assumed that

$$\frac{t_0 v^*}{L_0} = \varepsilon\,.$$

Concerning $\frac{t_0 j^*}{L_0 \varrho^* c^*}$ in the balance equation for c^ε, note that we assume the transition zone to be small even compared to the diameters of the pores. Since $\boldsymbol{j}$ and $\boldsymbol{j}^\varepsilon$ basically determine the thickness of this transition zone, the scaling factor should be at least of order ε^1:

$$\frac{t_0 j^*}{L_0 \varrho^* c^*} = \varepsilon\,.$$

Similarly, $\mathbb{T}^\varepsilon$ describes the interactions of the fluid inside the pores and we equally get

$$\frac{t_0 T^*}{L_0 \varrho^* v^*} = \varepsilon\,.$$

The dissipative energy flux, is a far reaching effect and behaves differently. In particular, we assume in the following that

$$\frac{t_0 h^*}{L_0 \varrho^* E^*} = 1\,.$$

Furthermore, for simplicity of notation, we drop the upper index $*$ in the differential operators div^*, ∇^* and ∂_t^* and obtain the following non dimensionalized set of equations in $\boldsymbol{Q}_1^\varepsilon$:

$$\begin{aligned}
\partial_t \left(\varrho^\varepsilon c^\varepsilon\right) + \varepsilon \mathrm{div}\, \left(\varrho^\varepsilon c^\varepsilon \boldsymbol{v}^\varepsilon\right) + \varepsilon \mathrm{div}\, \left(\boldsymbol{j}^\varepsilon\right) &= 0 \\
\partial_t \varrho^\varepsilon + \varepsilon \mathrm{div}\, \left(\varrho^\varepsilon \boldsymbol{v}^\varepsilon\right) &= 0 \\
\partial_t \left(\varrho^\varepsilon \boldsymbol{v}^\varepsilon\right) + \varepsilon \mathrm{div}\, \left(\varrho^\varepsilon \left(\boldsymbol{v}^\varepsilon \otimes \boldsymbol{v}^\varepsilon\right)\right) - \varepsilon \mathrm{div}\, \mathbb{T}^\varepsilon &= \boldsymbol{g}^\varepsilon \\
\partial_t \left(\varrho^\varepsilon E^\varepsilon\right) + \varepsilon \mathrm{div}\, \left(\varrho^\varepsilon E^\varepsilon \boldsymbol{v}^\varepsilon\right) - \mathrm{div}\, \boldsymbol{h}^\varepsilon &= \boldsymbol{g}^\varepsilon \cdot \boldsymbol{v}^\varepsilon\,,
\end{aligned} \tag{5.6}$$

where it is assumed that $\boldsymbol{j}^\varepsilon$ has its major impact on the porescale as well as $\mathbb{T}^\varepsilon$.

On $\boldsymbol{Q}_2^\varepsilon$, we apply a similar procedure to the balance of energy (4.4) and obtain

$$\partial E_2^\varepsilon - \mathrm{div}\, \boldsymbol{h}_2^\varepsilon = 0\,.$$

Finally, on Γ^ε, we obtain for balance of E_Γ and c the non dimensionalized equations

$$\partial_t E_\Gamma^\varepsilon - \varepsilon \mathrm{div}\, \boldsymbol{h}_\Gamma^\varepsilon = \overset{\oplus}{E}{}^\varepsilon$$
$$\varrho^\varepsilon \partial_t c^\varepsilon + \varepsilon \varrho^\varepsilon \boldsymbol{v}_\tau^\varepsilon \cdot \nabla_\tau c^\varepsilon = \overset{\oplus}{c}{}^\varepsilon .$$

Finally, remark that due to above non dimensionalization, also the material derivative becomes a scaled operator and one obtains the following important relations:

$$\dot{a} = \partial_t a + \varepsilon \boldsymbol{v}^\varepsilon \cdot \nabla a \qquad \text{for scalars } a\,, \tag{5.7}$$

$$\dot{\boldsymbol{a}} = \partial_t \boldsymbol{a} + \varepsilon \left(\nabla \boldsymbol{a}\right) \boldsymbol{v}^\varepsilon \quad \text{for vectors } \boldsymbol{a}\,, \tag{5.8}$$

$$\varrho^\varepsilon \dot{\overline{\nabla c^\varepsilon}} = \frac{\nabla \varrho^\varepsilon}{\varrho^\varepsilon} \left(\varepsilon \mathrm{div}\, \boldsymbol{j}_1^\varepsilon\right) - \varrho \left(\nabla c^\varepsilon\right)^T \left(\varepsilon \nabla \boldsymbol{v}^\varepsilon\right) - \mathrm{div}\, \left[\left(\varepsilon \mathrm{div}\, \boldsymbol{j}_1^\varepsilon\right) \mathbb{I}\right] , \tag{5.9}$$

where $\dot{\overline{\nabla c^\varepsilon}}$ denotes the material derivative of ∇c^ε and will be used in section 7.

6. The Assumption of Maximum Rate of Entropy Production

Following Callen [7], Heida, Málek and Rajagopal [23] and Heida [20], we assume the existence of entropy fields η^ε, η_2^ε and η_Γ^ε having the following properties:

- $\eta^\varepsilon = \tilde{\eta}(E^\varepsilon, \boldsymbol{v}^\varepsilon, \varrho^\varepsilon, c^\varepsilon, \nabla c^\varepsilon)$, $\eta_2^\varepsilon = \tilde{\eta}_2(E_2^\varepsilon)$, $\eta_\Gamma^\varepsilon = \tilde{\eta}_\Gamma(E_\Gamma^\varepsilon, c^\varepsilon, \nabla_\tau c^\varepsilon)$
- Keeping all other parameters fixed, $\tilde{\eta}$, $\tilde{\eta}_2$ and $\tilde{\eta}_\Gamma$ are strictly monotone increasing in E^ε, E_2^ε and E_Γ^ε respectively. Thus, $\tilde{\eta}(\cdot, \boldsymbol{v}, \varrho, c, \nabla c)$, $\tilde{\eta}_2(\cdot)$ and $\tilde{\eta}_\Gamma(\cdot, c, \nabla_\tau c)$ are invertible for fixed parameters and we can assume

$$E^\varepsilon = \tilde{E}(\eta^\varepsilon, \boldsymbol{v}^\varepsilon, \varrho^\varepsilon, c^\varepsilon, \nabla c^\varepsilon), \qquad E_2^\varepsilon = \tilde{E}_2(\eta_2^\varepsilon) \qquad \text{and} \qquad E_\Gamma^\varepsilon = \tilde{E}_\Gamma(\eta_\Gamma^\varepsilon, c^\varepsilon, \nabla_\tau c^\varepsilon) \tag{6.1}$$

- $0 \leq \vartheta^\varepsilon := \frac{\partial E^\varepsilon}{\partial \eta^\varepsilon}$, $0 \leq \vartheta_2^\varepsilon := \frac{\partial E_2^\varepsilon}{\partial \eta_2^\varepsilon}$ and $0 \leq \vartheta_\Gamma^\varepsilon := \frac{\partial E_\Gamma^\varepsilon}{\partial \eta_\Gamma^\varepsilon}$ are strictly increasing with E^ε, E_2^ε or E_Γ^ε respectively, where we will assume for simplicity, that all three quantities coincide on Γ. In particular, for the traces of ϑ^ε and ϑ_2^ε on Γ^ε holds

$$\vartheta^\varepsilon|_{\Gamma^\varepsilon} = \vartheta_2^\varepsilon|_{\Gamma^\varepsilon} = \vartheta_\Gamma^\varepsilon \qquad \text{on } \Gamma^\varepsilon\,. \tag{6.2}$$

  Thus, we denote all three quantities by ϑ^ε and call this quantity the *temperature* field of the system.

Having in mind (6.1), we calculate the material derivative of E and time derivatives of E_2 and E_Γ through:

$$\begin{aligned}
&\varrho^\varepsilon \dot{E}^\varepsilon = \varrho^\varepsilon \vartheta^\varepsilon \dot{\eta}^\varepsilon + \varrho^\varepsilon \frac{\partial E^\varepsilon}{\partial \boldsymbol{v}^\varepsilon} \cdot \dot{\boldsymbol{v}}^\varepsilon + \varrho^\varepsilon \frac{\partial E^\varepsilon}{\partial \varrho^\varepsilon} \dot{\varrho}^\varepsilon + \frac{\partial E^\varepsilon}{\partial c^\varepsilon} \dot{c}^\varepsilon + \frac{\partial E^\varepsilon}{\partial \left(\nabla c^\varepsilon\right)} \cdot \dot{\overline{\nabla c^\varepsilon}} && \text{on } \boldsymbol{Q}_1^\varepsilon\,,\\
&\partial_t E_2^\varepsilon = \vartheta^\varepsilon \partial_t \eta_2^\varepsilon && \text{on } \boldsymbol{Q}_2^\varepsilon\,,\\
&\partial_t E_\Gamma^\varepsilon = \vartheta^\varepsilon \partial_t \eta_\Gamma^\varepsilon + \frac{\partial E^\varepsilon}{\partial c^\varepsilon} \partial_t c^\varepsilon + \frac{\partial E^\varepsilon}{\partial \left(\nabla_\tau c^\varepsilon\right)} \cdot \partial_t \left(\nabla_\tau c^\varepsilon\right) && \text{on } \Gamma^\varepsilon\,.
\end{aligned} \tag{6.3}$$

Inserting (4.3), (4.4), (4.5), (4.6) and (5.9) into (6.3) yields new balance equations for η, η_2 and η_Γ of the form:

$$\begin{aligned}
\varrho^\varepsilon \dot{\eta}^\varepsilon &= \mathrm{div}\, \frac{\boldsymbol{q}^\varepsilon}{\vartheta^\varepsilon} + \frac{\xi^\varepsilon}{\vartheta^\varepsilon} \quad \text{on } \boldsymbol{Q}_1^\varepsilon\,,\\
\partial_t \eta_2^\varepsilon &= \mathrm{div}\, \frac{\boldsymbol{q}_2^\varepsilon}{\vartheta^\varepsilon} + \frac{\xi_2^\varepsilon}{\vartheta^\varepsilon} \quad \text{on } \boldsymbol{Q}_2^\varepsilon\,,\\
\partial_t \eta_\Gamma^\varepsilon &= \mathrm{div}_\tau \frac{\boldsymbol{q}_\Gamma^\varepsilon}{\vartheta^\varepsilon} + \frac{\xi_\Gamma^\varepsilon}{\vartheta^\varepsilon} \quad \text{on } \Gamma^\varepsilon\,,
\end{aligned}$$

where $\boldsymbol{q}_i^\varepsilon$ and ξ_i^ε will be provided below in section 7.

6.1. **Global Balance of Energy and Entropy.** For simplicity, we assume that $\boldsymbol{Q}$ is perfectly isolated, which means that any flux of mass, energy or entropy through $\partial\boldsymbol{Q}$ is excluded. Let $\boldsymbol{n}_{\partial\boldsymbol{Q}}$ be the outer normal vector of $\boldsymbol{Q}$, we thus obtain the following conditions on $\partial\boldsymbol{Q}$:

$$\begin{aligned} &\boldsymbol{h}^\varepsilon \cdot \boldsymbol{n}_{\partial\boldsymbol{Q}} = 0 && \boldsymbol{h}_2^\varepsilon \cdot \boldsymbol{n}_{\partial\boldsymbol{Q}} = 0 && \boldsymbol{h}_\Gamma^\varepsilon \cdot \boldsymbol{n}_{\partial\boldsymbol{Q}} = 0 \\ &\boldsymbol{q}^\varepsilon \cdot \boldsymbol{n}_{\partial\boldsymbol{Q}} = 0 && \boldsymbol{q}_2^\varepsilon \cdot \boldsymbol{n}_{\partial\boldsymbol{Q}} = 0 && \boldsymbol{q}_\Gamma^\varepsilon \cdot \boldsymbol{n}_{\partial\boldsymbol{Q}} = 0 \\ &\boldsymbol{j}_1^\varepsilon \cdot \boldsymbol{n}_{\partial\boldsymbol{Q}} = 0 && \boldsymbol{v} = \boldsymbol{0} \end{aligned} \tag{6.4}$$

Furthermore, it will be assumed that there is no net mass flux through the boundary Γ^ε, nor any chemical reaction at the boundary, i.e.

$$\boldsymbol{v}^\varepsilon \cdot \boldsymbol{n}_{\Gamma^\varepsilon} = 0 \qquad \text{and} \qquad \boldsymbol{j}_1 \cdot \boldsymbol{n}_{\Gamma^\varepsilon} = 0 \qquad \text{on } \Gamma^\varepsilon\,. \tag{6.5}$$

The total energy $\mathcal{E}^\varepsilon$ and total entropy $\mathcal{S}^\varepsilon$ of the system are given as the integral of the respective fields on $\boldsymbol{Q}_1^\varepsilon$, $\boldsymbol{Q}_2^\varepsilon$ and Γ^ε:

$$\mathcal{E}^\varepsilon = \int_{\boldsymbol{Q}_1^\varepsilon} \varrho^\varepsilon E^\varepsilon + \int_{\boldsymbol{Q}_2^\varepsilon} E_2^\varepsilon + \varepsilon \int_{\Gamma^\varepsilon} E_\Gamma^\varepsilon\,, \tag{6.6}$$

$$\mathcal{S}^\varepsilon = \int_{\boldsymbol{Q}_1^\varepsilon} \varrho^\varepsilon \eta^\varepsilon + \int_{\boldsymbol{Q}_2^\varepsilon} \eta_2^\varepsilon + \varepsilon \int_{\Gamma^\varepsilon} \eta_\Gamma^\varepsilon\,, \tag{6.7}$$

where the boundary integrals are assumed to enter of order ε since

$$\lim_{\varepsilon\to 0} \varepsilon \int_{\Gamma^\varepsilon} 1\,dx = \int_{\boldsymbol{Q}} \int_{\Gamma} 1\,dx\,dy\,.$$

Note that this can be realized by choosing appropriate scales for E_Γ^* and η_Γ^*. Global changes of energy are assumed to be only due to work done by body forces. In particular, the global balance of energy reads:

$$\begin{aligned} 0 = \frac{d}{dt}\mathcal{E}^\varepsilon - \int_{\boldsymbol{Q}_1^\varepsilon} \boldsymbol{g}^\varepsilon \cdot \boldsymbol{v}^\varepsilon &= \int_{\boldsymbol{Q}_1^\varepsilon} \varrho^\varepsilon \dot{E}^\varepsilon + \int_{\boldsymbol{Q}_2^\varepsilon} \partial_t E_2^\varepsilon + \varepsilon \int_{\Gamma^\varepsilon} \partial_t E_\Gamma^\varepsilon - \int_{\boldsymbol{Q}_1^\varepsilon} \boldsymbol{g}^\varepsilon \cdot \boldsymbol{v}^\varepsilon \\ &= \varepsilon \int_{\Gamma^\varepsilon} \left(\frac{1}{\varepsilon} (\boldsymbol{h}^\varepsilon - \boldsymbol{h}_2^\varepsilon) \cdot \boldsymbol{n}_{\Gamma^\varepsilon} + \varepsilon \mathrm{div}_\tau \boldsymbol{h}_\Gamma^\varepsilon + \overset{\oplus}{E}{}^\varepsilon \right). \end{aligned} \tag{6.8}$$

Due to (6.4) and lemma 1 holds

$$\int_{\Gamma^\varepsilon} \mathrm{div}_\tau \boldsymbol{h}_\Gamma^\varepsilon = \int_{\partial\boldsymbol{Q}\cap\Gamma^\varepsilon} \boldsymbol{h}_\Gamma^\varepsilon \cdot \boldsymbol{n}_{\partial\boldsymbol{Q}} = 0\,,$$

and due to the reasons pointed out in [20], equation (6.8) implies the local energy conservation[2]

$$\frac{1}{\varepsilon} (\boldsymbol{h}^\varepsilon - \boldsymbol{h}_2^\varepsilon) \cdot \boldsymbol{n}_{\Gamma^\varepsilon} + \overset{\oplus}{E}{}^\varepsilon = 0\,. \tag{6.9}$$

The time derivative of global entropy with respect to time yields:

$$\begin{aligned} \Xi^\varepsilon := \frac{d}{dt}\mathcal{S}^\varepsilon &= \int_{\boldsymbol{Q}_1^\varepsilon} \frac{\xi^\varepsilon}{\vartheta^\varepsilon} + \int_{\boldsymbol{Q}_2^\varepsilon} \frac{\xi_2^\varepsilon}{\vartheta^\varepsilon} + \varepsilon \int_{\Gamma^\varepsilon} \left(\frac{1}{\varepsilon\,\vartheta^\varepsilon} (\boldsymbol{q}^\varepsilon - \boldsymbol{q}_2^\varepsilon) \cdot \boldsymbol{n}_{\Gamma^\varepsilon} + \frac{\xi_\Gamma^\varepsilon}{\vartheta^\varepsilon} \right) \\ &= \int_{\boldsymbol{Q}_1^\varepsilon} \frac{\xi^\varepsilon}{\vartheta^\varepsilon} + \int_{\boldsymbol{Q}_2^\varepsilon} \frac{\xi_2^\varepsilon}{\vartheta^\varepsilon} + \varepsilon \int_{\Gamma^\varepsilon} \frac{\xi_{\Gamma,tot}^\varepsilon}{\vartheta^\varepsilon}\,, \end{aligned} \tag{6.10}$$

[2]We shortly repeat the original argumentation with slightly modified formulas: As pointed out in [20], "*the reason why* $div_\tau \boldsymbol{h}_\Gamma^\varepsilon$ *does not appear in* (6.9) *is twofold: First, due to lemma 1, it is possible to add* $\int_\Gamma \varepsilon\, div_\tau \boldsymbol{f}_\tau$ *of any tangential vector field* $\boldsymbol{f}_\tau$ *in* (6.8) *without violating the equality. In particular, we could equally derive a condition* $\frac{1}{\varepsilon} (\boldsymbol{h}^\varepsilon - \boldsymbol{h}_2^\varepsilon) \cdot \boldsymbol{n}_{\Gamma^\varepsilon} + \overset{\oplus}{E}{}^\varepsilon + r\varepsilon\, div_\tau \boldsymbol{h}_\Gamma^\varepsilon = 0$ *for any* $r \in \mathbb{R}$*. Second, it is reasonable to assume that absorption is a local process, i.e. that the energy supply* $\boldsymbol{h}^\varepsilon \cdot \boldsymbol{n}_{\Gamma^\varepsilon}$ *is first absorbed by* Γ^ε *through* $\overset{\oplus}{E}{}^\varepsilon$ *and then dissipated through* $\boldsymbol{h}_\Gamma^\varepsilon$*, instead of being directly dissipated through* $\boldsymbol{h}_\Gamma^\varepsilon$."

where the second law of thermodynamics requires

$$\Xi^\varepsilon \geq 0\,. \tag{6.11}$$

Note that $\frac{1}{\varepsilon\,\vartheta^\varepsilon}\,(\boldsymbol{q}^\varepsilon - \boldsymbol{q}_2^\varepsilon)\cdot\boldsymbol{n}_{\Gamma^\varepsilon}$, the exchange of entropy between $\boldsymbol{Q}_1^\varepsilon$, $\boldsymbol{Q}_2^\varepsilon$ and Γ^ε, contributes to the production of entropy, itself.

6.2. **The Assumption of Maximum Rate of Entropy Production.** It was the idea of Rajagopal and Srinivasa [39] to make use of ξ^ε in order to derive constitutive equations in the bulk using an assumption of maximum rate of entropy production. This idea was generalized by the author to ξ_Γ^ε [19, 20] and Heida, Málek and Rajagopal [21], i.e. to lower dimensional structures.

Being aware of the loss of generality, it is assumed that (6.11) can be split up into the local conditions

$$\begin{aligned} \xi^\varepsilon \geq 0 \quad &\text{pointwise in } \boldsymbol{Q}_1^\varepsilon\,, & \xi_2^\varepsilon \geq 0 \quad &\text{pointwise in } \boldsymbol{Q}_2^\varepsilon\,,\\ \xi_{\Gamma,tot}^\varepsilon \geq 0 \quad &\text{pointwise on } \Gamma^\varepsilon\,. \end{aligned}$$

The local rates of entropy production ξ^ε, ξ_2^ε and ξ_Γ^ε will be assumed to have the form

$$\begin{aligned} \xi^\varepsilon &= \sum_\alpha J_\alpha^\varepsilon \cdot f_\alpha(\boldsymbol{A}^\varepsilon)\\ \xi_2^\varepsilon &= \sum_\beta J_\beta^\varepsilon \cdot f_\beta(\boldsymbol{A}_2^\varepsilon)\\ \xi_\Gamma^\varepsilon &= \sum_\gamma J_{\gamma,\Gamma}^\varepsilon \cdot f_{\gamma,\Gamma}(\boldsymbol{A}_\Gamma^\varepsilon) \end{aligned}$$

where J_*^ε are the thermodynamical fluxes on $\boldsymbol{Q}_1^\varepsilon$, $\boldsymbol{Q}_2^\varepsilon$ or Γ^ε respectively and $\boldsymbol{A}^\varepsilon$, $\boldsymbol{A}_2^\varepsilon$ and $\boldsymbol{A}_\Gamma^\varepsilon$ are the relevant thermodynamical affinities. In our context, the thermodynamical fluxes are given through $\mathbb{T}^\varepsilon$, $\boldsymbol{j}^\varepsilon$, $\boldsymbol{h}^\varepsilon$, $\boldsymbol{q}^\varepsilon$ and similar quantities on $\boldsymbol{Q}_2^\varepsilon$ and Γ^ε, while the affinities are the unknowns of the system, such as ϱ^ε, c^ε, $\boldsymbol{v}^\varepsilon$ and ϑ^ε. For a more detailed explanation of thermodynamical fluxes and affinities, refer to [20, 23].

In what follows, we assume that the rates of entropy production on $\boldsymbol{Q}_1^\varepsilon$, $\boldsymbol{Q}_2^\varepsilon$ and Γ^ε are locally given by $\tilde{\xi}^\varepsilon$, $\tilde{\xi}_2^\varepsilon$ and $\tilde{\xi}_\Gamma^\varepsilon$. In particular, $\tilde{\xi}^\varepsilon$, $\tilde{\xi}_2^\varepsilon$ and $\tilde{\xi}_\Gamma^\varepsilon$ depend on the fluxes via:

$$\xi^\varepsilon = \tilde{\xi}^\varepsilon\left((J_\alpha^\varepsilon)_\alpha\right), \qquad \xi_2^\varepsilon = \tilde{\xi}_2^\varepsilon\left(\left(J_{2,\alpha}^\varepsilon\right)_\alpha\right), \qquad \xi_\Gamma^\varepsilon = \tilde{\xi}_\Gamma^\varepsilon\left((J_{\beta,\Gamma})_\beta\right).$$

We then maximize $\tilde{\xi}^\varepsilon$, $\tilde{\xi}_2^\varepsilon$ and $\tilde{\xi}_\Gamma^\varepsilon$ with respect to the local constraints

$$\tilde{\xi}^\varepsilon = \sum_\alpha J_\alpha^\varepsilon \cdot f_\alpha^\varepsilon(\boldsymbol{A}^\varepsilon)\,, \qquad \tilde{\xi}_2^\varepsilon = \sum_\alpha J_{2,\alpha}^\varepsilon \cdot f_{2,\alpha}^\varepsilon(\boldsymbol{A}_2^\varepsilon) \qquad \text{and} \qquad \tilde{\xi}_\Gamma^\varepsilon = \sum_\beta J_{\beta,\Gamma}^\varepsilon \cdot f_{\beta,\Gamma}^\varepsilon(\boldsymbol{A}_\Gamma^\varepsilon)\,. \tag{6.12}$$

According to the theory of Lagrange multipliers, the last problem is equivalent with finding λ_1^ε such that

$$\frac{\partial\tilde{\xi}^\varepsilon}{\partial J_\alpha^\varepsilon} + \lambda_1^\varepsilon\left(\frac{\partial\tilde{\xi}^\varepsilon}{\partial J_\alpha^\varepsilon} - f_\alpha^\varepsilon(\boldsymbol{A}^\varepsilon)\right) = 0 \quad\Leftrightarrow\quad f_\alpha^\varepsilon(\boldsymbol{A}^\varepsilon) = \frac{1+\lambda_1^\varepsilon}{\lambda_1^\varepsilon}\frac{\partial\tilde{\xi}^\varepsilon}{\partial J_\alpha^\varepsilon} \quad \forall\alpha\,. \tag{6.13}$$

and similarly we find λ_2^ε on $\boldsymbol{Q}_1^\varepsilon$ with

$$\frac{\partial\tilde{\xi}_2^\varepsilon}{\partial J_{2,\alpha}^\varepsilon} + \lambda_2^\varepsilon\left(\frac{\partial\tilde{\xi}_2^\varepsilon}{\partial J_{2,\alpha}^\varepsilon} - f_{2,\alpha}^\varepsilon(\boldsymbol{A}_2^\varepsilon)\right) = 0 \quad\Leftrightarrow\quad f_{2,\alpha}^\varepsilon(\boldsymbol{A}_2^\varepsilon) = \frac{1+\lambda_2^\varepsilon}{\lambda_2^\varepsilon}\frac{\partial\tilde{\xi}_2^\varepsilon}{\partial J_{2,\alpha}^\varepsilon} \quad \forall\alpha\,.$$

and λ_Γ for the boundary problem:

$$\frac{\partial\tilde{\xi}_\Gamma^\varepsilon}{\partial J_{\beta,\Gamma}^\varepsilon} + \lambda_\Gamma^\varepsilon\left(\frac{\partial\tilde{\xi}_\Gamma^\varepsilon}{\partial J_{\beta,\Gamma}^\varepsilon} - f_{\beta,\Gamma}^\varepsilon(\boldsymbol{A}_\Gamma^\varepsilon)\right) = 0 \quad\Leftrightarrow\quad f_{\beta,\Gamma}^\varepsilon(\boldsymbol{A}_\Gamma^\varepsilon) = \frac{1+\lambda_\Gamma^\varepsilon}{\lambda_\Gamma^\varepsilon}\frac{\partial\tilde{\xi}_\Gamma^\varepsilon}{\partial J_{\beta,\Gamma}^\varepsilon} \quad \forall\beta\,. \tag{6.14}$$

In the present work, only the simple quadratic case for $\tilde{\xi}$ and $\tilde{\xi}_\Gamma$ will be studied

$$\tilde{\xi}^\varepsilon(J_\alpha^\varepsilon) = \sum_\alpha \frac{1}{\gamma_\alpha} |J_\alpha^\varepsilon|^2 , \quad \tilde{\xi}_2^\varepsilon(J_{2,\alpha}^\varepsilon) = \sum_\alpha \frac{1}{\gamma_{2,\alpha}} \left|J_{2,\alpha}^\varepsilon\right|^2 , \quad \tilde{\xi}_\Gamma^\varepsilon(J_{\beta,\Gamma}^\varepsilon) = \sum_\beta \frac{1}{\gamma_{\beta,\Gamma}} \left|J_{\beta,\Gamma}^\varepsilon\right|^2$$

which yields together with (6.13) and (6.14)

$$J_\alpha^\varepsilon = \gamma_\alpha^\varepsilon f_\alpha^\varepsilon (\boldsymbol{A}^\varepsilon) , \qquad J_{2,\alpha}^\varepsilon = \gamma_{2,\alpha}^\varepsilon f_{2,\alpha}^\varepsilon (\boldsymbol{A}_2^\varepsilon) , \qquad J_{\beta,\Gamma}^\varepsilon = \gamma_{\beta,\Gamma}^\varepsilon f_{\beta,\Gamma}^\varepsilon (\boldsymbol{A}_\Gamma^\varepsilon) . \tag{6.15}$$

Note that similar to [20] we can also immediately pass to $\tilde{\xi}^\varepsilon$, $\tilde{\xi}_2^\varepsilon$ and $\tilde{\xi}_\Gamma^\varepsilon$ being quadratic positive definite bilinear forms.

7. The Complete Microscopic Model

7.1. **Physical assumptions.** We will now derive the microscopic model for two constituent flow in porous media. As already mentioned in the introduction, we assume for simplicity, that the fluids under consideration are water and air and that the transition zone is thin compared to the pore diameter. Note that the considerations below will not consider phase transitions like evaporation, condensation, freezing or thawing. We also do not account for any deformation of the solid matrix, in particular we exclude swelling processes, such that the domains $\boldsymbol{Q}_1^\varepsilon$ as well as $\boldsymbol{Q}_2^\varepsilon$ are not changing with time.

7.2. **The pore space.** We directly start from system (5.6), assuming that the energy is given through

$$\begin{aligned} E^\varepsilon = E(\boldsymbol{v}^\varepsilon, \varrho^\varepsilon, \eta^\varepsilon, c^\varepsilon, \nabla c^\varepsilon) &= \frac{1}{2} |\boldsymbol{v}^\varepsilon|^2 + \tilde{E}(\eta^\varepsilon, \varrho^\varepsilon, c^\varepsilon) + \hat{E}(\varrho^\varepsilon, \nabla c^\varepsilon) , \\ \text{with} \qquad \hat{E}(\varrho^\varepsilon, \nabla c^\varepsilon) &= \frac{1}{2\varrho^\varepsilon} \varepsilon^2 \sigma |\nabla c^\varepsilon|^2 . \end{aligned} \tag{7.1}$$

Note that the characteristic scale of energy E^* and velocity v^* are connected with each other, through

$$E^\varepsilon = \frac{1}{2} \frac{(v^*)^2}{E^*} |\boldsymbol{v}^\varepsilon|^2 + \cdots ,$$

implying the assumption $\frac{(v^*)^2}{E^*} = 1$.

The scaling ε^2 in $\hat{E}$ reflects the assumption that the interfacial energy $\varepsilon^2\sigma$ and the resulting diffusive smoothing of the interface have their major impact on a scale which is much smaller than the macro scale and the scale of energy.

Starting from (6.3), using (5.6) and (7.1) and introducing the notations

$$p^\varepsilon := (\varrho^\varepsilon)^2 \frac{\partial E^\varepsilon}{\partial \varrho^\varepsilon} \qquad \mu^\varepsilon := \frac{\partial E^\varepsilon}{\partial c^\varepsilon} \qquad \partial_z E^\varepsilon := \frac{\partial E^\varepsilon}{\partial (\nabla c^\varepsilon)} .$$

we obtain for the local balance of entropy in $\boldsymbol{Q}_1^\varepsilon$

$$\varrho^\varepsilon \dot{\eta^\varepsilon} - \operatorname{div} \frac{\boldsymbol{q}^\varepsilon}{\vartheta} = \xi^\varepsilon ,$$

where, following [20, 23], the rate of entropy production ξ^ε and the heat flux $\boldsymbol{q}^\varepsilon$ can be identified as

$$\xi^\varepsilon = \varepsilon(\mathbb{T}^\varepsilon + \mathbb{T}_c^\varepsilon) \cdot \mathbb{D}\boldsymbol{v}^\varepsilon + \frac{\boldsymbol{q}^\varepsilon}{\vartheta^\varepsilon} \cdot \nabla \vartheta^\varepsilon + p^\varepsilon \varepsilon \operatorname{div} \boldsymbol{v}^\varepsilon - \varepsilon \boldsymbol{j}_1^\varepsilon \cdot \nabla (\mu_c^\varepsilon + \mu^\varepsilon) , \tag{7.2}$$

$$\boldsymbol{q}^\varepsilon = \varepsilon (\mu_c^\varepsilon + \mu^\varepsilon) \boldsymbol{j}_1^\varepsilon + \varepsilon \partial_z E^\varepsilon \operatorname{div} \boldsymbol{j}_1^\varepsilon + \boldsymbol{h}^\varepsilon - \varepsilon \mathbb{T}^\varepsilon \boldsymbol{v}^\varepsilon , \tag{7.3}$$

with

$$\mu_c^\varepsilon := -\operatorname{div} (\partial_z E^\varepsilon) - \partial_z E^\varepsilon \frac{\nabla \varrho^\varepsilon}{\varrho^\varepsilon} \qquad \text{and} \qquad \mathbb{T}_c^\varepsilon := \left(\sigma \varepsilon^2 \nabla c^\varepsilon \otimes \nabla c^\varepsilon\right) . \tag{7.4}$$

Finally, define $m^\varepsilon := \frac{1}{3}\mathrm{tr}\,(\mathbb{T}^\varepsilon + \mathbb{T}_c^\varepsilon)$ and $\mathbb{S}^\varepsilon := \mathbb{T}^\varepsilon + \mathbb{T}_c^\varepsilon - m^\varepsilon \mathbb{I}$ to obtain

$$\xi^\varepsilon = \varepsilon \mathbb{S}^\varepsilon \cdot \mathbb{D}\boldsymbol{v}^\varepsilon + \frac{\boldsymbol{q}^\varepsilon}{\vartheta} \cdot \nabla\vartheta + (m^\varepsilon + p^\varepsilon)\,\varepsilon \mathrm{div}\,\boldsymbol{v}^\varepsilon - \varepsilon \boldsymbol{j}_1^\varepsilon \cdot \nabla\,(\mu_c^\varepsilon + \mu^\varepsilon)\ .$$

Now, in order to apply the assumption of maximum rate of entropy production, let ξ^ε be given through

$$\xi^\varepsilon = \tilde{\xi}^\varepsilon(\mathbb{S}^\varepsilon, (m^\varepsilon + p^\varepsilon), \boldsymbol{q}^\varepsilon, \boldsymbol{j}_1^\varepsilon) = \frac{1}{\nu^\varepsilon}\,|\mathbb{S}^\varepsilon|^2 + \frac{3}{\nu^\varepsilon + 3\lambda^\varepsilon}\,(m^\varepsilon + p^\varepsilon)^2 + \frac{1}{\kappa_1^\varepsilon \vartheta^\varepsilon}\,|\boldsymbol{q}^\varepsilon|^2 + \frac{1}{J^\varepsilon}\,|\boldsymbol{j}_1^\varepsilon|^2\ .$$

Then, maximizing $\tilde{\xi}^\varepsilon$ with respect to

$$\tilde{\xi}^\varepsilon = \varepsilon \mathbb{S}^\varepsilon \cdot \mathbb{D}\boldsymbol{v}^\varepsilon + \frac{\boldsymbol{q}^\varepsilon}{\vartheta} \cdot \nabla\vartheta + (m^\varepsilon + p^\varepsilon)\,\varepsilon \mathrm{div}\,\boldsymbol{v}^\varepsilon - \varepsilon \boldsymbol{j}_1^\varepsilon \cdot \nabla\,(\mu_c^\varepsilon + \mu^\varepsilon)$$

leads to the resulting set of constitutive equations:

$$\begin{aligned}
\mathbb{T}^\varepsilon &= -\varepsilon\nu^\varepsilon \mathbb{D}\boldsymbol{v}^\varepsilon - \varepsilon\lambda^\varepsilon \mathrm{div}\,\boldsymbol{v}^\varepsilon \mathbb{I} + p^\varepsilon \mathbb{I} + \sigma\varepsilon^2 \nabla c^\varepsilon \otimes \nabla c^\varepsilon\,,\\
\boldsymbol{j}_1^\varepsilon &= -\varepsilon J^\varepsilon \left(\nabla\mu^\varepsilon - \varepsilon^2\sigma\nabla\Delta c^\varepsilon\right)\,,\\
\boldsymbol{h}^\varepsilon &= \kappa_1^\varepsilon \nabla\vartheta^\varepsilon - \varepsilon\,(\mu_c^\varepsilon + \mu^\varepsilon)\,\boldsymbol{j}_1^\varepsilon - \partial_z E\,[\varepsilon \mathrm{div}\,\boldsymbol{j}_1^\varepsilon] + \varepsilon \mathbb{T}^\varepsilon \boldsymbol{v}^\varepsilon\,,
\end{aligned}$$

and the full system in $\boldsymbol{Q}_1^\varepsilon$ reads:

$$\begin{aligned}
\partial_t\,(\varrho^\varepsilon c^\varepsilon) + \varepsilon \mathrm{div}\,(\varrho^\varepsilon c^\varepsilon \boldsymbol{v}^\varepsilon) - \varepsilon^2 J^\varepsilon \mathrm{div}\,\left(\nabla\mu^\varepsilon - \varepsilon^2\sigma\nabla\Delta c^\varepsilon\right) &= 0\\
\partial_t \varrho^\varepsilon + \varepsilon \mathrm{div}\,(\varrho^\varepsilon \boldsymbol{v}^\varepsilon) &= 0\\
\partial_t\,(\varrho^\varepsilon \boldsymbol{v}^\varepsilon) + \varepsilon \mathrm{div}\,(\varrho^\varepsilon\,(\boldsymbol{v}^\varepsilon \otimes \boldsymbol{v}^\varepsilon)) - \varepsilon^2 \mathrm{div}\,(\nu^\varepsilon \mathbb{D}\boldsymbol{v}^\varepsilon) + \varepsilon\nabla\,(p^\varepsilon - \varepsilon\lambda^\varepsilon \mathrm{div}\,\boldsymbol{v}^\varepsilon)&\\
+\varepsilon \mathrm{div}\,\left(\sigma\varepsilon^2 \nabla c^\varepsilon \otimes \nabla c^\varepsilon\right) &= \boldsymbol{g}^\varepsilon\\
\partial_t\,(\varrho^\varepsilon E^\varepsilon) + \varepsilon \mathrm{div}\,(\varrho^\varepsilon E^\varepsilon \boldsymbol{v}^\varepsilon) - \mathrm{div}\,(\kappa_1 \nabla\vartheta^\varepsilon - \varepsilon\,(\mu_c^\varepsilon + \mu^\varepsilon)\,\boldsymbol{j}_1^\varepsilon)&\\
-\mathrm{div}\,(-\partial_z E\,[\varepsilon \mathrm{div}\,\boldsymbol{j}_1^\varepsilon] + \varepsilon \mathbb{T}^\varepsilon \boldsymbol{v}^\varepsilon) &= \boldsymbol{g}^\varepsilon \cdot \boldsymbol{v}^\varepsilon\,.
\end{aligned} \tag{7.5}$$

Note that the parameters ν^ε, λ^ε, J^ε or κ_1^ε may depend on the variables ϱ^ε, c^ε, or ϑ^ε. This will be important for the asymptotic expansion of κ_1^ε, while for the other constants, this is not of importance in the formal calculations.

7.3. **A remark on scaling of pressure.** Comparing with former papers by Allaire on derivation of Darcy's law from Stokes equation [4, 27], we could expect ∇p^ε to appear of order ε^0 instead of ε^1. However, note that in [4, 27], p^ε is an unknown, due to incompressibility, and corresponds to $\frac{1}{3}\mathrm{tr}\mathbb{T}^\varepsilon$. Thus, incompressibility replaces thermodynamical pressure p^ε by the Lagrange multiplier $\frac{1}{3}\mathrm{tr}\mathbb{T}^\varepsilon$. For the present approach holds: fixing $\mathrm{div}\,\boldsymbol{v}^\varepsilon = 0$, no $\frac{1}{3}\mathrm{tr}\mathbb{T}^\varepsilon$ becomes unknown. In case no apriori condition is imposed on $\mathrm{div}\,\boldsymbol{v}^\varepsilon$, we find

$$\frac{3}{\nu^\varepsilon + 3\lambda^\varepsilon}\,(m^\varepsilon + p^\varepsilon) = \mathrm{div}\,\boldsymbol{v}^\varepsilon$$

where p^ε is thermodynamical pressure and thus a derived quantity.

7.4. **The soil matrix.** Since the soil matrix is a rigid body, we drop the balances of mass and momentum and focus on the balance of energy, which reads

$$\partial_t E_2^\varepsilon - \mathrm{div}\,\boldsymbol{h}_2^\varepsilon = 0 \quad \text{on } \boldsymbol{Q}_2^\varepsilon\,, \tag{7.6}$$

where E_2^ε is the energy per volume in $\boldsymbol{Q}_2^\varepsilon$ and $\boldsymbol{h}_2^\varepsilon$ is the corresponding heat flux. If the constitutive assumption for E_2^ε takes the form

$$E_2^\varepsilon = \tilde{E}_2^\varepsilon(\eta_2^\varepsilon)$$

with η_2^ε the entropy per volume in $\boldsymbol{Q}_2^\varepsilon$, and if it is assumed that $\vartheta^\varepsilon = \frac{\partial E_2^\varepsilon}{\partial \eta_2^\varepsilon}$, we easily find

$$\partial_t \eta_2^\varepsilon - \operatorname{div} \frac{\boldsymbol{q}_2^\varepsilon}{\vartheta^\varepsilon} = \boldsymbol{q}_2^\varepsilon \cdot \frac{\nabla \vartheta^\varepsilon}{\vartheta^\varepsilon} \,,$$

where

$$\boldsymbol{q}_2^\varepsilon = \boldsymbol{h}_2^\varepsilon = \kappa_2^\varepsilon \nabla \vartheta^\varepsilon \,. \tag{7.7}$$

In order to connect the balance of energy on $\boldsymbol{Q}_1^\varepsilon$ and $\boldsymbol{Q}_2^\varepsilon$ we need to take a closer look on the boundary Γ^ε.

7.5. **Boundary conditions.** Following [20], we start from the following abstract boundary conditions[3] on Γ^ε:

$$\begin{aligned} \varrho^\varepsilon \partial_t c^\varepsilon + \varepsilon \varrho^\varepsilon \boldsymbol{v}_\tau^\varepsilon \cdot \nabla_\tau c^\varepsilon &= \overset{\oplus}{c}{}^\varepsilon \\ \partial_t E_\Gamma^\varepsilon - \varepsilon \operatorname{div}_\tau \boldsymbol{h}_\Gamma^\varepsilon &= \overset{\oplus}{E}{}^\varepsilon \end{aligned} \tag{7.8}$$

where ϱ^ε and c^ε are the traces on Γ^ε of the corresponding fields in $\boldsymbol{Q}_1^\varepsilon$, $\boldsymbol{v}_\tau^\varepsilon$ is the tangential part of $\boldsymbol{v}^\varepsilon$ on Γ^ε, E_Γ^ε is the surface energy on Γ^ε, i.e. energy per area of Γ^ε, $\boldsymbol{h}_\Gamma^\varepsilon$ is the surface heat flux and $\overset{\oplus}{E}{}^\varepsilon$ is the rate of energy exchange between Γ^ε and $\boldsymbol{Q}_1^\varepsilon$, respectively $\boldsymbol{Q}_2^\varepsilon$.

In order to proceed, consider the following constitutive assumption on the local surface energy density E_Γ^ε:

$$E_\Gamma^\varepsilon = E_{\Gamma,0}^\varepsilon(\eta_\Gamma^\varepsilon) + F_\Gamma(c^\varepsilon) + \frac{1}{2}\varepsilon^2 \sigma_\Gamma \left|\nabla_\tau c^\varepsilon\right|^2 \tag{7.9}$$

where F_Γ is assumed to be independent on ε with

$$f_\Gamma^\varepsilon := \partial_c F_\Gamma(c^\varepsilon)$$

and make use of the fact that

$$\partial_t E_\Gamma^\varepsilon = \vartheta^\varepsilon \partial_t \eta_\Gamma^\varepsilon + \frac{\partial E_\Gamma^\varepsilon}{\partial c^\varepsilon} \partial_t c^\varepsilon + \frac{\partial E_\Gamma^\varepsilon}{\partial \varrho^\varepsilon} \partial_t \varrho^\varepsilon$$

using assumption (6.2), we follow [20] and obtain

$$\begin{aligned} \partial_t \eta_\Gamma^\varepsilon &= \frac{1}{\vartheta^\varepsilon} \left(\varepsilon \boldsymbol{q}_\Gamma^\varepsilon \cdot \frac{\nabla_\tau \vartheta^\varepsilon}{\vartheta^\varepsilon} + \overset{\oplus}{E}{}^\varepsilon - \boldsymbol{v}_\tau \cdot \left[-\varepsilon \varrho^\varepsilon \mu_{\Gamma,2}^\varepsilon \nabla_\tau c^\varepsilon \right] - \mu_{\Gamma,2}^\varepsilon \overset{\oplus}{c}{}^\varepsilon \right) + \varepsilon \operatorname{div}_\tau \left(\frac{\boldsymbol{q}_\Gamma^\varepsilon}{\vartheta^\varepsilon} \right) \\ \boldsymbol{q}_\Gamma^\varepsilon &= \boldsymbol{h}_\Gamma^\varepsilon - \varepsilon \sigma_\Gamma \nabla_\tau c^\varepsilon \, \partial_t c^\varepsilon \,, \end{aligned} \tag{7.10}$$

where

$$\mu_{\Gamma,2}^\varepsilon = \left(\frac{f_\Gamma^\varepsilon}{\varrho^\varepsilon} - \frac{1}{\varrho^\varepsilon} \varepsilon^2 \sigma_\Gamma \Delta_{\tau\tau} c^\varepsilon \right) \quad .$$

The total rate of entropy production then reads:

$$\frac{d}{dt}\mathcal{S} := \int_{\boldsymbol{Q}_1^\varepsilon} \left(\frac{\xi^\varepsilon}{\vartheta^\varepsilon} + \operatorname{div} \boldsymbol{q}^\varepsilon \right) + \int_{\boldsymbol{Q}_2^\varepsilon} \left(\frac{\xi_2^\varepsilon}{\vartheta^\varepsilon} + \operatorname{div} \boldsymbol{q}_2^\varepsilon \right) + \varepsilon \int_{\partial\Gamma} \partial_t \eta_\Gamma^\varepsilon \,.$$

Using partial integration as well as (7.3), (7.7), (6.5) and (7.10), the last equality can be rewritten as

$$\frac{d}{dt}\mathcal{S} = \int_{\boldsymbol{Q}_1^\varepsilon} \frac{\xi^\varepsilon}{\vartheta^\varepsilon} + \int_{\boldsymbol{Q}_2^\varepsilon} \frac{\xi_2^\varepsilon}{\vartheta^\varepsilon} + \int_{\partial\Gamma} \frac{\varepsilon}{\vartheta^\varepsilon} \left[\boldsymbol{q}_\Gamma^\varepsilon \cdot \frac{\varepsilon \nabla_\tau \vartheta^\varepsilon}{\vartheta^\varepsilon} - \boldsymbol{v}_\tau^\varepsilon \cdot \left(\check{\mathbb{T}}_\tau^\varepsilon + \mu_{\boldsymbol{v},\Gamma}^\varepsilon \right) - \mu_{\Gamma,c}^\varepsilon \overset{\oplus}{c}{}^\varepsilon \right] \,,$$

[3] In [20], the author also suggests different approaches to boundary conditions. However, the approach chosen in the present calculations is most easy to handle and calculations for different abstract form of boundary conditions may be performed similarly, following the presented outline.

where $\check{\mathbb{T}}^\varepsilon_\tau := (\mathbb{T}^\varepsilon \boldsymbol{n}_{\Gamma^\varepsilon})_\tau$ is the tangential part of the surface stress $\mathbb{T}^\varepsilon \boldsymbol{n}_{\Gamma^\varepsilon}$ and

$$\mu^\varepsilon_{\boldsymbol{v},\Gamma} = -\varrho^\varepsilon \mu^\varepsilon_{\Gamma,2} \varepsilon \nabla_\tau c^\varepsilon \qquad \mu^\varepsilon_{\Gamma,c} = \left(\mu^\varepsilon_{\Gamma,2} + \partial_z \hat{u}^\varepsilon \cdot \boldsymbol{n}_{\Gamma^\varepsilon}\right) \quad , \tag{7.11}$$

These equations yield the final constitutive equations

$$\begin{aligned} \check{\mathbb{T}}^\varepsilon_\tau &= -\alpha_\Gamma \boldsymbol{v}^\varepsilon_\tau - \mu^\varepsilon_{\boldsymbol{v},\Gamma} \\ \varrho^\varepsilon \partial_t c^\varepsilon + \varepsilon \varrho^\varepsilon \boldsymbol{v}^\varepsilon \cdot \nabla_\tau c^\varepsilon = \overset{\oplus}{c}{}^\varepsilon &= \beta^*_\Gamma \left(\frac{\sigma_\Gamma}{\varrho^\varepsilon} \varepsilon^2 \Delta_\tau c^\varepsilon - \frac{\mu^\varepsilon_\Gamma}{\varrho^\varepsilon} - \varepsilon \sigma \nabla c^\varepsilon \cdot \boldsymbol{n}_{\Gamma^\varepsilon} \right) \\ \boldsymbol{q}^\varepsilon_\Gamma &= \kappa_\Gamma \varepsilon \nabla_\tau \vartheta^\varepsilon \\ \overset{\oplus}{E} + \frac{1}{\varepsilon} (\boldsymbol{h}^\varepsilon - \boldsymbol{h}^\varepsilon_2) \cdot \boldsymbol{n}_{\Gamma^\varepsilon} &= 0 \,. \end{aligned} \tag{7.12}$$

8. Formal Asymptotic Expansion

We will now perform a formal asymptotic expansion of system (7.5) and (7.6) together with boundary conditions (7.12). To this aim, we expand η^ε, η^ε_2, η^ε_Γ, ϱ^ε, c^ε, $\boldsymbol{v}^\varepsilon$, ϑ^ε and p^ε according to (3.2) by

$$a^\varepsilon(t,\cdot) = \sum_{i=0}^{\infty} \varepsilon^i a_i(t,\cdot,\frac{\cdot}{\varepsilon})$$

and define for any $\phi \in C^1([0,T] \times \boldsymbol{Q} \times \boldsymbol{Y})$

$$D_t^{0,y}\phi := \partial_t \phi + \boldsymbol{v}_0 \cdot \nabla_y \phi \quad \text{or} \quad D_t^{0,xy}\phi := \partial_t \phi + \varepsilon \boldsymbol{v}_0 \cdot \nabla_x \phi + \boldsymbol{v}_0 \cdot \nabla_y \phi \,.$$

Formal asymptotic expansion yields for any such ϕ with $\phi^\varepsilon(t,\cdot) := \phi(t,\cdot,\frac{\cdot}{\varepsilon})$:

$$\dot{\phi^\varepsilon} \to D_t^{0,y}\phi \qquad \text{as} \quad \varepsilon \to 0 \,. \tag{8.1}$$

However, it is desirable to have macroscopic convective fluxes in the limit equations. Thus, we keep the terms $\varepsilon \boldsymbol{v}_0 \cdot \nabla_x \phi$ and replace $D_t^{0,y}$ by $D_t^{0,xy}$ in a sense that we replace (8.1) in the asymptotic expansion by

$$\dot{\phi^\varepsilon} \rightsquigarrow D_t^{0,xy}\phi \qquad \text{as} \quad \varepsilon \to 0 \,.$$

This approach is further justified by improved formal error estimates, as shown in appendix B.

Note that in all experiments, a macroscopic pressure gradient is found either balancing macroscopic gravitational forces or causing a net macroscopic mass transport. Thus, for similar reason as for the conservation of macroscopic flow field, it is reasonable to keep the macroscopic pressure gradient $\varepsilon \nabla_x p_0$ in the limit equations. As stated in section 7, the parameters ν, λ, J or κ_1 may depend on the variables ϱ^ε, c^ε, or ϑ^ε. Thus, we would formally also have to use an expansion for these parameters. However, except for κ_1, only the first order of the expanded coefficient is relevant for the limit equations. For κ_1, we will need the expansion up to order 2:

$$\kappa_1^\varepsilon = \kappa_1 + \varepsilon \kappa_{1,1} + \varepsilon^2 \kappa_{1,2} + \mathcal{O}(\varepsilon^3)$$

and similarly also for κ_2^ε.

The zero order approximating system then reads

$$\begin{aligned} D_t^{0,xy}\varrho_0 + \varrho_0 \mathrm{div}_y\, \boldsymbol{v}_0 + \varepsilon \varrho_0 \mathrm{div}_x\, \boldsymbol{v}_0 &= 0 \\ \varrho_0 D_t^{0,xy} c_0 - \mathrm{div}_y\, (\nabla_y \mu_0 - \sigma \nabla_y \Delta_{yy} c_0) &= 0 \\ \varrho_0 D_t^{0,xy} \boldsymbol{v}_0 - \mathrm{div}_y\, (\nu \mathbb{D}_y \boldsymbol{v}_0) + \nabla_y (p_0 - \lambda \mathrm{div}_y\, \boldsymbol{v}_0) + \varepsilon \nabla_x p_0 + \mathrm{div}_y\, (\sigma \nabla_y c_0 \otimes \nabla_y c_0) &= \boldsymbol{g}_0 \\ \varrho_0 D_t^{0,xy} E_0 + \mathrm{div}_y \left((\mu_c + \mu)\, \boldsymbol{j}_{1,0} + \partial_z E_0 \left[\mathrm{div}_y\, \boldsymbol{j}_{1,0}\right] - \mathbb{T}_0 \boldsymbol{v}_0 \right) & \\ - \mathrm{div}_x\, (\kappa_1 \nabla_x \vartheta_0 + \kappa_1 \nabla_y \vartheta_1 + \kappa_{1,1} \nabla_y \vartheta_0) & \\ - \mathrm{div}_y\, (\kappa_1 \nabla_x \vartheta_1 + \kappa_1 \nabla_y \vartheta_2 + \kappa_{1,1} \nabla_y \vartheta_1 + \kappa_{1,1} \nabla_x \vartheta_0 + \kappa_{1,2} \nabla_y \vartheta_0) - \boldsymbol{g}_0 \cdot \boldsymbol{v}_0 &= 0 \,, \end{aligned} \tag{8.2}$$

where we assumed $\kappa_1 = const$ for simplicity. Here, the homogenized stress tensor $\mathbb{T}_0$, and the other quantities E_0, μ_0, $\boldsymbol{j}_{1,0}$and p_0 are given through

$$\mathbb{T}_0 = -\nu\mathbb{D}_y\boldsymbol{v}_0 + (p_0 + \lambda \mathrm{div}_y\, \boldsymbol{v}_0)\,\mathbb{I} + \sigma\nabla_y c_0 \otimes \nabla_y c_0,$$
$$E = E_0(\eta_0, \varrho_0, c_0) + \frac{1}{2}\,|\boldsymbol{v}_0|^2 + \frac{\sigma}{2\varrho_0}\,|\nabla_y c_0|^2$$

and

$$\mu_0 = \frac{\partial E_0}{\partial c_0}, \quad \boldsymbol{j}_{1,0} = -J\,(\nabla_y\mu_0 - \sigma\nabla_y\Delta_{yy}c_0) \quad \text{and} \quad p_0 = \varrho_0^2\frac{\partial E_0}{\partial \varrho_0}\,. \tag{8.3}$$

Additionally, we find the following equations of order ε^{-1} and ε^{-2} on $\boldsymbol{Q}\times\boldsymbol{Y}_1$:

$$\begin{aligned} \mathrm{div}_y\,(\kappa_1\nabla_y\vartheta_0) &= 0\\ \mathrm{div}_y\,(\kappa_1\nabla_x\vartheta_0 + \kappa_1\nabla_y\vartheta_1 + \kappa_{1,1}\nabla_y\vartheta_0) + \mathrm{div}_x\,(\kappa_1\nabla_y\vartheta_0) &= 0\,. \end{aligned} \tag{8.4}$$

The microscopic boundary conditions finally read

$$\partial_t E_{\Gamma,0} - \mathrm{div}_{\tau,y}\,\boldsymbol{h}_{\Gamma,0} = \overset{\oplus}{E}$$
$$\varrho_0\partial_t c_0 + \varrho_0\boldsymbol{v}_0\nabla_{\tau,y}c_0 = \overset{\oplus}{c}_0$$

with a constitutive equation

$$E_{\Gamma,0} = E_\Gamma(\eta_{\Gamma,0}) + F_\Gamma(c_0) + \frac{\sigma_\Gamma}{2}\,|\nabla_{\tau,y}c_0|^2$$

and the resulting two-scale constitutive equations.

$$\begin{aligned} \check{\mathbb{T}}_{\tau,0} &= -\alpha_\Gamma\boldsymbol{v}_\tau - \varrho_0\left(\frac{\sigma_\Gamma}{\varrho_0}\Delta_{\tau\tau,yy}c_0 - \frac{f_\Gamma(c_0)}{\varrho_0}\right)\nabla_{\tau,y}c_0\\ \overset{\oplus}{c}_0 &= \beta_\Gamma^*\left(\frac{\sigma_\Gamma}{\varrho_0}\Delta_{\tau\tau,yy}c_0 - \frac{f_\Gamma(c_0)}{\varrho_0} - \sigma\nabla_y c_0\cdot\boldsymbol{n}_\Gamma\right)\\ \boldsymbol{q}_{\Gamma,0} &= 2\kappa\frac{\nabla_\tau\vartheta}{\vartheta} = \boldsymbol{h}_{\Gamma,0} - \sigma_\Gamma\nabla_{\tau,y}c_0\,\partial_t c_0\,. \end{aligned} \tag{8.5}$$

$$\begin{aligned} \overset{\oplus}{E} = &-(\boldsymbol{h}_0 - (\kappa_1-\kappa_2)\,\nabla_x\vartheta_1 - (\kappa_1-\kappa_2)\,\nabla_y\vartheta_2)\cdot\boldsymbol{n}_\Gamma\\ &+((\kappa_{1,1}-\kappa_{2,1})\,(\nabla_y\vartheta_1 + \nabla_x\vartheta_0) + (\kappa_{1,2}-\kappa_{2,2})\,\nabla_y\vartheta_0)\cdot\boldsymbol{n}_\Gamma \end{aligned}$$

where

$$\check{\mathbb{T}}_{\tau,0} = (\mathbb{T}_0\boldsymbol{n}_\Gamma)_\tau = ((\nu\mathbb{D}_y\boldsymbol{v}_0 - \sigma\nabla_y c_0\otimes\nabla_y c_0)\,\boldsymbol{n}_\Gamma)_\tau$$

is the tangential part of the surface stress vector and

$$\boldsymbol{h}_0 = (\mu_c + \mu)\,\boldsymbol{j}_{1,0} + \partial_z E\left[\mathrm{div}_y\,\boldsymbol{j}_{1,0}\right] - \mathbb{T}_0\boldsymbol{v}_0\,.$$

The first equation of (8.5) is but some generalized Navier-Slip condition on the microscale and the second equation is the dynamic boundary condition for Cahn-Hilliard fluids.

The boundary conditions of order ε^{-1} and ε^{-2} which stem from $(7.12)_4$ read

$$\begin{aligned} (\kappa_1\nabla_y\vartheta_0 - \kappa_2\nabla_y\vartheta_0)\cdot\boldsymbol{n}_\Gamma &= 0\,,\\ ((\kappa_1-\kappa_2)\,\nabla_y\vartheta_1 + (\kappa_1-\kappa_2)\,\nabla_x\vartheta_0 + (\kappa_{1,1}-\kappa_{2,1})\,\nabla_y\vartheta_0)\cdot\boldsymbol{n}_\Gamma &= 0\,. \end{aligned} \tag{8.6}$$

On $\boldsymbol{Q}_2\times\boldsymbol{Y}$, the balance of energy splits up into

$$\begin{aligned} \partial_t E_2 - \mathrm{div}_x\,(\kappa_2\nabla_x\vartheta_0 + \kappa_2\nabla_y\vartheta_1 + \kappa_{2,1}\nabla_y\vartheta_0)&\\ -\mathrm{div}_y\,(\kappa_2\nabla_x\vartheta_1 + \kappa_2\nabla_y\vartheta_2 + \kappa_{2,1}\nabla_y\vartheta_1 + \kappa_{2,1}\nabla_x\vartheta_0 + \kappa_{2,2}\nabla_y\vartheta_0) &= 0\\ \mathrm{div}_y\,(\kappa_2\nabla_y\vartheta_0) &= 0\\ \mathrm{div}_y\,(\kappa_2\nabla_x\vartheta_0 + \kappa_2\nabla_y\vartheta_1 + \kappa_{2,1}\nabla_y\vartheta_0) + \mathrm{div}_x\,(\kappa_2\nabla_y\vartheta_0) &= 0\,, \end{aligned} \tag{8.7}$$

where

$$E_2 = \tilde{E}_2(\eta_{2,0})$$

9. Some Important Remarks on Effective Macroscopic Equations

The two-scale model as such already is the solution we were searching for. Therefore, before going into the details of the derivation of effective macroscopic equations, remark that it is not the aim of the following two sections to derive explicit macroscopic equations that replace the obtained two-scale model. It is also not possible to calculate the macroscopic permeabilities without knowing the solutions of the two-scale model. Rather, it is the aim of the following calculations to investigate the macroscopic behavior of the solutions of the two-scale model.

Thus, in all calculations below in sections 10 and 11, it will be assumed that there is a solution

$$(\varrho_0, c_0, \boldsymbol{v}_0, E_0, \vartheta_0, \vartheta_1, \vartheta_2)$$

that solves the two-scale problem (8.2) with the corresponding constitutive assumptions from section 8. Then, the macroscopic behavior of this solution will be derived by averaging the equations over $\boldsymbol{Y}$.

10. Macroscopic Balance Equations of Mass and Energy

10.1. **Mass balance equations.** We will extract the information on the macroscopic transport of air and water from the mixture's velocity field using the total momenta and total masses of both constituents in the pore space. With regard to section 4.1, water is characterized by $c_0 = 1$ and air by $c_0 = 0$. Then, macroscopic partial density $\overline{\varrho}_w$ and macroscopic velocity $\bar{\boldsymbol{v}}_w$ of water are given through

$$\bar{\varrho}_w = \int_{\boldsymbol{Y}} (c_0 \varrho_0) \qquad\qquad \bar{\boldsymbol{v}}_w = \frac{1}{\bar{\varrho}_w} \int_{\boldsymbol{Y}} (c_0 \varrho_0 \boldsymbol{v}_0 + j_{c,0}) \tag{10.1a}$$

Since the diffusive flux $\boldsymbol{j}_{c,0}$ is restricted to the thin transition zone, it has no major effect on the total water flux on the macro scale. Thus, we assume

$$\bar{\boldsymbol{v}}_w = \frac{1}{\bar{\varrho}_w} \int_{\boldsymbol{Y}} (c_0 \varrho_0 \boldsymbol{v}_0) \tag{10.1b}$$

Analogously, one obtains for the velocity $\bar{\boldsymbol{v}}_a$ and density $\bar{\varrho}_a$ of air:

$$\overline{\varrho}_a := \int_{\boldsymbol{Y}} ((1-c_0)\varrho_0)\ , \qquad\qquad \bar{\boldsymbol{v}}_a := \frac{1}{\bar{\varrho}_a} \int_{\boldsymbol{Y}} ((1-c_0)\varrho_0 \boldsymbol{v}_0)\ . \tag{10.2}$$

Since the abstract mass balance equations read according to (8.2) and (8.3)

$$\begin{aligned} \partial_t (\varrho_0 c_0) + \operatorname{div}_y (\varrho_0 c_0 \boldsymbol{v}_0) + \varepsilon \operatorname{div}_x (\varrho_0 c_0 \boldsymbol{v}_0) + \operatorname{div}_y \boldsymbol{j}_0 = 0 \\ \partial_t (\varrho_0 (1-c_0)) + \operatorname{div}_y (\varrho_0 (1-c_0) \boldsymbol{v}_0) + \varepsilon \operatorname{div}_x (\varrho_0 (1-c_0) \boldsymbol{v}_0) - \operatorname{div}_y \boldsymbol{j}_0 = 0\,, \end{aligned}$$

integrating these equations in the periodic coordinate over $\boldsymbol{Y}_1$ will cause all terms $\operatorname{div}_y(\dots)$ to vanish and we obtain:

$$\partial_t \bar{\varrho}_w + \varepsilon \operatorname{div}_x (\bar{\varrho}_w \bar{\boldsymbol{v}}_w) = 0 \tag{10.3a}$$

$$\partial_t \bar{\varrho}_a + \varepsilon \operatorname{div}_x (\bar{\varrho}_a \bar{\boldsymbol{v}}_a) = 0\,. \tag{10.3b}$$

Taking a look on section 3.1,we hope to find representations

$$\boldsymbol{v}_{w,0} := c_0 \boldsymbol{v}_0 = \hat{\boldsymbol{v}}_w + \tilde{\boldsymbol{v}}_w \qquad \boldsymbol{v}_{a,0} := (1-c_0)\,\boldsymbol{v}_0 = \hat{\boldsymbol{v}}_a + \tilde{\boldsymbol{v}}_a$$

with $\tilde{\boldsymbol{v}}_i$ given through

$$\tilde{\boldsymbol{v}}_i = \int_0^t \sum_j \left[\partial_t \left(\boldsymbol{g} - \nabla_x p_0\right)_j (s,x)\right] \boldsymbol{u}_j(t-s,y) ds\,.$$

This will be topic of section 11.

10.2. **Macroscopic balance of energy.** Having a look on (8.4), (8.6) and $(8.7)_{2,3}$, we find

$$\begin{aligned}\operatorname{div}_y\left(\kappa_1\nabla_y\vartheta_0\right)&=0\quad\text{on }\boldsymbol{Q}\times\boldsymbol{Y}_1\\ \operatorname{div}_y\left(\kappa_2\nabla_y\vartheta_0\right)&=0\quad\text{on }\boldsymbol{Q}\times\boldsymbol{Y}_2\\ \left(\kappa_1\nabla_y\vartheta_0-\kappa_2\nabla_y\vartheta_0\right)\cdot\boldsymbol{n}_\Gamma&=0\quad\text{on }\boldsymbol{Q}\times\Gamma\,,\end{aligned}$$

and thus $\nabla_y\vartheta_0\equiv 0$. Therefore, equations $(8.4)_2$, $(8.6)_2$ and $(8.7)_3$ yield

$$\operatorname{div}_y\left(\kappa_1\nabla_x\vartheta_0+\kappa_1\nabla_y\vartheta_1\right)=0\quad\text{on }\boldsymbol{Q}\times\boldsymbol{Y}_1\,, \tag{10.4a}$$

$$\operatorname{div}_y\left(\kappa_2\nabla_x\vartheta_0+\kappa_2\nabla_y\vartheta_1\right)=0\quad\text{on }\boldsymbol{Q}\times\boldsymbol{Y}_2\,, \tag{10.4b}$$

$$\left(\left(\kappa_1-\kappa_2\right)\nabla_y\vartheta_1+\left(\kappa_1-\kappa_2\right)\nabla_x\vartheta_0\right)\cdot\boldsymbol{n}_\Gamma=0\quad\text{on }\boldsymbol{Q}\times\Gamma\,, \tag{10.4c}$$

which holds in case

$$\vartheta_1=\sum_{i=1}^{3}\phi_i\partial_i\vartheta_0$$

where the ϕ_i are solutions to a decoupled cell problem:

$$\begin{aligned}\operatorname{div}_y\left(\kappa_1\nabla_y\phi_i+\kappa_1\boldsymbol{e}_i\right)&=0\quad\text{on }Y_1\text{ for all }x\\ \operatorname{div}_y\left(\left(\kappa_2\nabla_y\phi_i+\kappa_2\boldsymbol{e}_i\right)\right.&=0\quad\text{on }Y_2\text{ for all }x\\ \left(\kappa_1\left(\nabla_y\phi_i+\boldsymbol{e}_i\right)-\kappa_2\left(\nabla_y\phi_i+\boldsymbol{e}_i\right)\right)\cdot\boldsymbol{n}_\Gamma&=0\quad\text{on }\Gamma\text{ for all }x\end{aligned} \tag{10.5}$$

In line with (6.6), the macroscopic energy per volume is defined as

$$\mathcal{E}=\int_{\boldsymbol{Y}_1}\varrho_0E+\int_{\boldsymbol{Y}_2}E_{2,0}+\int_\Gamma E_\Gamma\,.$$

Then, equations $(8.2)_4$ and $(8.7)_1$ together with $(8.5)_4$ integrated over $\boldsymbol{Y}$ simply yield

$$\partial_t\mathcal{E}+\varepsilon\operatorname{div}_x\int_{\boldsymbol{Y}_1}\left(\boldsymbol{v}_0\varrho_0E\right)-\operatorname{div}_x\left(\kappa^{hom}\nabla_x\vartheta_0\right)=\int_{\boldsymbol{Y}_1}\boldsymbol{g}\cdot\boldsymbol{v}_0\quad\text{on }\boldsymbol{Q}$$

where the properties of ϕ_i as solutions of (10.5) yield:

$$\kappa_{ij}^{hom}:=\int_{\boldsymbol{Y}_1}\left(\nabla_y\phi_i+\boldsymbol{e}_i\right)\cdot\left(\kappa_1\left(\nabla_y\phi_j+\boldsymbol{e}_j\right)\right)+\int_{\boldsymbol{Y}_2}\left(\nabla_y\phi_i+\boldsymbol{e}_i\right)\cdot\left(\kappa_2\left(\nabla_y\phi_j+\boldsymbol{e}_j\right)\right)\,.$$

If it is assumed that $\boldsymbol{g}$ is the gravitational force

$$\boldsymbol{g}=\hat{\boldsymbol{g}}\varrho_0\,,$$

with the gravitational acceleration constant $\hat{\boldsymbol{g}}$ and using the notations introduced above in (10.1) and (10.2), the macroscopic balance of energy simply reads

$$\partial_t\mathcal{E}+\varepsilon\operatorname{div}_x\int_{\boldsymbol{Y}_1}\left(\boldsymbol{v}_0\varrho_0E\right)-\operatorname{div}_x\left(\kappa^{hom}\nabla_x\vartheta_0\right)=\bar{\varrho}_w\hat{\boldsymbol{g}}\cdot\bar{\boldsymbol{v}}_w+\bar{\varrho}_a\hat{\boldsymbol{g}}\cdot\bar{\boldsymbol{v}}_a\quad\text{on }\boldsymbol{Q}\,.$$

11. Decoupling of Phases: Macroscopic Permeability Tensors

As stated in section 9, the two-scale system, which was obtained in section 8 as such already is a solution of the homogenization problem, meaning that it is a first order approximation, which accounts for all important microscopic and macroscopic effects. However, since the common approach to two-phase flow in porous media is based on macroscopic transport equations (10.3) with constitutive equations

$$\begin{aligned}\bar{\boldsymbol{v}}_w&=A_w(\rho_w\boldsymbol{g}-\nabla p_w)\\ \bar{\boldsymbol{v}}_a&=A_a(\rho_a\boldsymbol{g}-\nabla p_a)\,,\end{aligned}$$

we will demonstrate that such equations can be obtained from the two-scale model in section 8.

Therefore, in what follows, the two scale equation (8.2) with boundary condition $(8.5)_1$ will be separated into two macroscopic equations for the water and air velocities. The result will yield approximate formulas for the dependence of macroscopic permeabilities on the microscopic geometry and the dynamic changing of this geometry. However, note that we will not discuss the existence of a capillary pressure, nor its dependence on saturation. For a very short and rough treatment of capillary pressure, refer to the next section 12. Since the calculations are formal and we use heuristic approximations, it is possible that numerical simulations will show that more effects have to be taken into account.

Clearly, physics at the transition zone is different from physics outside of the transition zone. In particular, capillary effects have their major impact on the flow field close to the transition zone. Thus we will develop a formalism to split up the two-scale model into equations at the transition zone and equations in the pure water and air regions. This will help to find effective permeability tensors for both fluids. The resulting permeability tensors will then account for microscopic geometry and its evolution.

11.1. **Assumptions on the geometry.** Note that the phase field model does not explicitly separate water and air transport, while sharp interface models and classical macroscopic models do. Thus, in order to proceed, it is necessary to split the cell $\boldsymbol{Y}_1$ and the microscopic domain $\boldsymbol{Q}_1^\varepsilon$ into the regions that are occupied by air and water respectively. Since we also have to capture interactions between air and water, we also have to introduce an "interfacial region", which is related to the transition zone. Note that the geometry is given by a smooth phase field and it therefore makes no sense to characterize air, water and interface by classical characteristic functions attaining only the values 0 and 1. Instead, smoothed characteristic functions for air, water and the interface will be constructed.

To be more concrete assume that there are constants

$$0 < a_0 < a_1 < b_1 < b_0 < 1$$

and smooth functions ϖ_a, ϖ_w, ϖ_I with

$$\varpi_a(c) = \begin{cases} 1 & \text{for } c < a_0 \\ \exp\left(-\frac{(a_0-c)^2}{(c-a_1)^2}\right) & \text{for } c \in [a_0, a_1] \\ 0 & \text{for } c > a_1 \end{cases}, \quad \varpi_w(c) = \begin{cases} 1 & \text{for } c > b_0 \\ \exp\left(-\frac{(b_1-c)^2}{(c-b_0)^2}\right) & \text{for } c \in [b_1, b_0] \\ 0 & \text{for } c < b_1 \end{cases}$$

as well as

$$\varpi_I(c) = 1 - (\varpi_a(c) + \varpi_w(c)) \,.$$

Then, the characteristic function of the air phase, the water phase and the interfacial region are defined by

$$\chi_a^\varepsilon(x) := \varpi_a(c^\varepsilon(x)), \quad \chi_w^\varepsilon(x) := \varpi_w(c^\varepsilon(x)), \quad \chi_I^\varepsilon(x) := \varpi_I(c^\varepsilon(x)) \,,$$

and we find

$$\chi_w^\varepsilon + \chi_a^\varepsilon + \chi_I^\varepsilon = 1 \,.$$

The formal asymptotic expansions of these functions read

$$\chi_*^\varepsilon(x) = \varpi_*(c_0(x, \frac{x}{\varepsilon})) + \varepsilon \varpi_*'(c_0(x, \frac{x}{\varepsilon}))\, c_1(x, \frac{x}{\varepsilon}) + \mathcal{O}(\varepsilon^2) \qquad \text{for } * = a, w, I \,,$$

or, equivalently:

$$\chi_*^\varepsilon(x) = \chi_{*,0}(x, \frac{x}{\varepsilon}) + \varepsilon \chi_{*,1}(x, \frac{x}{\varepsilon}) + \mathcal{O}(\varepsilon^2) \qquad \text{for } * = a, w, I \,,$$

where the definition of the $\chi_{*,i}$ are given implicitly by comparison and we note that

$$\chi_{w,0} + \chi_{a,0} + \chi_{I,0} = 1 \,. \tag{11.1}$$

Based on these smoothed characteristic functions, the three regions $\boldsymbol{Y}_a$, $\boldsymbol{Y}_w$ and $\boldsymbol{Y}_I$ are introduced through:

$$\boldsymbol{Y}_*(x) = \{y \in \boldsymbol{Y}_1 \,:\, \chi_{*,0}(x,y) > 0\} \qquad \text{for } * = a, w, I\,,$$

which are the regions that are mostly occupied by air or water and the interfacial region $\boldsymbol{Y}_I$ in the cell $\boldsymbol{Y}_1$.

Note that $\boldsymbol{Y}_1 = \boldsymbol{Y}_a \cup \boldsymbol{Y}_w \cup \boldsymbol{Y}_I$ and $\boldsymbol{Y}_a \cap \boldsymbol{Y}_w = \emptyset$ but $\boldsymbol{Y}_a \cap \boldsymbol{Y}_I \neq \emptyset$ and $\boldsymbol{Y}_w \cap \boldsymbol{Y}_I \neq \emptyset$. Furthermore, for any $\varepsilon > 0$, we can introduce the sets $\boldsymbol{Q}_a^\varepsilon$, $\boldsymbol{Q}_w^\varepsilon$ and $\boldsymbol{Q}_I^\varepsilon$ through

$$\boldsymbol{Q}_*^\varepsilon(x) = \{y \in \boldsymbol{Q}_1 \,:\, \chi_*^\varepsilon(x) > 0\} \qquad \text{for } * = a, w, I\,,,$$

11.2. **Assumptions on the coefficients p^ε, $\boldsymbol{g}^\varepsilon$ and ϱ^ε.** We will restart from the microscopic balance of momentum $(7.5)_3$. We assume that the densities of of water ρ_w and air ρ_a do not vary much over the porescale, such that for these two density fields and an interfacial residual density $\tilde{\varrho}$ such that we find:

$$\varrho^\varepsilon(x) = \chi_a^\varepsilon(x)\,\rho_A(x) + \chi_w^\varepsilon(x)\,\rho_W(x) + \chi_I^\varepsilon(x)\,\tilde{\varrho}(x, c^\varepsilon(x)) + \mathcal{O}(\varepsilon)\,, \tag{11.2a}$$

as well as

$$\varrho_0(x,y) = \chi_a(x,y)\rho_A(x) + \chi_w(x,y)\rho_W(x) + \chi_I(x,y)\tilde{\varrho}(x, c_0(x,y)) \tag{11.2b}$$

for the limit two-scale density field ϱ_0. Here, ρ_A and ρ_W are some functions

$$\rho_A\,,\, \rho_W : \quad \boldsymbol{Q} \to \mathbb{R}_{>0}$$

with $\rho_A < \rho_W$, representing the macroscopic density fields of air and water and

$$\begin{aligned} \tilde{\varrho} : \quad & \boldsymbol{Q} \times [0,1] \to \mathbb{R}_{>0} \\ & (x,c) \mapsto \tilde{\varrho}(x,c) \in [\rho_A(x), \rho_W(x)] \end{aligned}$$

is the c-dependent density distribution in $\boldsymbol{Y}_I$ or $\boldsymbol{Q}_I^\varepsilon$[4]. The body force is assumed to be due to gravitation and therefore reads

$$\boldsymbol{g}^\varepsilon = \varrho^\varepsilon \boldsymbol{g}\,.$$

Since the pressure is given through (compare for (8.3))

$$p^\varepsilon = (\varrho^\varepsilon)^2\,\frac{\partial E}{\partial \varrho^\varepsilon}, \quad \text{respectively} \quad p_0 = (\varrho_0)^2\,\frac{\partial E}{\partial \varrho_0}\,,$$

assumption (11.2) suggests to split p^ε into

$$\begin{aligned} p^\varepsilon &= \tilde{p}_a^\varepsilon + \tilde{p}_w^\varepsilon + \tilde{p}_I^\varepsilon \\ \varepsilon\nabla p^\varepsilon &= \chi_a^\varepsilon(x)\varepsilon\nabla\left(\tilde{p}_a^\varepsilon + \tilde{p}_I^\varepsilon\right) + \chi_w^\varepsilon(x)\varepsilon\nabla\left(\tilde{p}_w^\varepsilon + \tilde{p}_I^\varepsilon\right) + \chi_I^\varepsilon\varepsilon\nabla\left(\tilde{p}_I^\varepsilon + \tilde{p}_a^\varepsilon + \tilde{p}_w^\varepsilon\right)\,, \end{aligned}$$

where

$$\tilde{p}_a^\varepsilon := \chi_a^\varepsilon p^\varepsilon, \quad \tilde{p}_w^\varepsilon := \chi_w^\varepsilon p^\varepsilon \quad \text{and} \quad \tilde{p}_I := \chi_I^\varepsilon p^\varepsilon\,.$$

[4]Clearly, these assumptions on ϱ imply a kind of "incompressibility" in y, which enters the system aposteriori. However, the way this assumption enters, it is no limitation to the two-scale model but simplifies the present calculations. An a-priori assumption on incompressibility of water and air would have made it necessary to work within the framework of quasi-incompressible mixtures, see [23].

Using a formal asymptotic expansion ansatz

$$
\begin{aligned}
\tilde{p}_a^\varepsilon(x) &= \tilde{p}_a(x) + \sum_{i=1}^{\infty} \varepsilon \tilde{p}_{a,i}(x, \frac{x}{\varepsilon}) \\
\tilde{p}_w^\varepsilon(x) &= \tilde{p}_w(x) + \sum_{i=1}^{\infty} \varepsilon \tilde{p}_{w,i}(x, \frac{x}{\varepsilon}) \\
\tilde{p}_I^\varepsilon(x) &= \tilde{p}_I(x, \frac{x}{\varepsilon}) + \sum_{i=1}^{\infty} \varepsilon \tilde{p}_{I,i}(x, \frac{x}{\varepsilon}) \,,
\end{aligned}
\tag{11.3}
$$

the resulting two-scale model would read according to section 8:

$$
\begin{aligned}
\varrho_0 D_t^{0,*} \boldsymbol{v}_0 - \operatorname{div}_y \left(\nu \mathbb{D}_y \boldsymbol{v}_0\right) - \nabla_y \left(\lambda \operatorname{div}_y \boldsymbol{v}_0\right) + \chi_a \varepsilon \nabla_x \left(\tilde{p}_a + \tilde{p}_I\right) + \chi_w \varepsilon \nabla_x \left(p_w + \tilde{p}_I\right) \\
+ \chi_I \nabla_y \left(\tilde{p}_I + \varepsilon \tilde{p}_{a,1} + \varepsilon \tilde{p}_{w,1}\right) + \operatorname{div}_y \left(\sigma \nabla_y c_0 \otimes \nabla_y c_0\right) + \mathcal{O}(\varepsilon^2) = \boldsymbol{g} \varrho_0 \,.
\end{aligned}
\tag{11.4}
$$

In particular, $\tilde{p}_a$, $\tilde{p}_w$, $\tilde{p}_I$ and p_0 are related by

$$
p_0 = \tilde{p}_a + \tilde{p}_w + \tilde{p}_I \,.
$$

In what follows, for simplicity of notation, we introduce

$$
p_k = \varepsilon \tilde{p}_k \qquad \text{and} \qquad p_{k,i} = \varepsilon \tilde{p}_{k,i} \qquad \forall k \in \{a, w\} \,.
$$

11.3. **The relations between ρ_a and $\bar{\varrho}_a$ and between ρ_w and $\bar{\varrho}_w$.** Comparing the quantities ρ_A and $\bar{\varrho}_a$ and ρ_W and $\bar{\varrho}_w$, we see that ρ_a and ρ_w are the physical densities of water and air at point $x \in \boldsymbol{Q}$ while the quantities $\bar{\varrho}_a$ and $\bar{\varrho}_w$ are the physical densities multiplied by the volume fractions which are occupied by air and water respectively. Thus, since $\chi_w \approx c_0$ and $\chi_a \approx (1 - c_0)$ except for the transition zone, we find with

$$
\Phi_a := \int_{\boldsymbol{Y}} \chi_a, \qquad \Phi_w := \int_{\boldsymbol{Y}} \chi_w
$$

the relations

$$
\bar{\varrho}_a \approx \int_{\boldsymbol{Y}_1} \chi_a \rho_A = \Phi_a \rho_A \qquad\qquad \bar{\varrho}_w \approx \int_{\boldsymbol{Y}_1} \chi_w \rho_W = \Phi_w \rho_W
$$

11.4. **Formal decoupling.** Equations $(7.5)_3$, respectively (11.4) describe the evolution of the velocity field of the whole mixture. However, as stated above, we are interested in separating air and water transport and thus in those parts of the velocity field $\boldsymbol{v}_0$ which belong to $c_0 \approx 1$ and $c_0 \approx 0$.

This is achieved splitting up the velocity field $\boldsymbol{v}_0$ into the velocities $\boldsymbol{v}_{0,a}$ of air, of water $\boldsymbol{v}_{0,w}$ and of the interface $\boldsymbol{v}_{0,I}$:

$$
\boldsymbol{v}_{0,a} := \chi_a \boldsymbol{v}_0, \quad \boldsymbol{v}_{0,w} := \chi_w \boldsymbol{v}_0 \quad \text{and} \quad \boldsymbol{v}_{0,I} := \chi_I \boldsymbol{v}_0 \,,
\tag{11.5}
$$

with

$$
\boldsymbol{v}_{0,a} + \boldsymbol{v}_{0,w} + \boldsymbol{v}_{0,I} = \boldsymbol{v}_0 \,.
$$

Also, we multiply each of the terms

$$
\partial_t(\varrho_0 \boldsymbol{v}_0), \quad \operatorname{div}_y \left(\nu \nabla_y \boldsymbol{v}_0\right), \quad \nabla_y \left(\lambda \operatorname{div}_y \boldsymbol{v}_0\right), \quad \operatorname{div}_y \left(\mathbb{T}_{c0}\right), \quad \varrho_0 \boldsymbol{g}
$$

with (11.1) and reorganize the equation in terms of $\chi_{w,0}$, $\chi_{a,0}$, and $\chi_{I,0}$ to obtain

$$
\begin{aligned}
(11.6)\quad & \chi_{a,0}\Big(\partial_t(\varrho_0\boldsymbol{v}_{0,a}) - \mathrm{div}_y\,(\nu\nabla_y\boldsymbol{v}_{0,a}) - \nabla_y\,(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,a}) + \nabla_y p_{a,1} + \nabla_x p_a - \rho_a\boldsymbol{g}\Big)\\
&\quad + \chi_{a,0}\Big(\partial_t(\varrho_0\boldsymbol{v}_{0,I}) - \mathrm{div}_y\,(\nu\nabla_y\boldsymbol{v}_{0,I}) - \nabla_y\,(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,I}) + \mathrm{div}_y\,(\mathbb{T}_{c0})\Big)\\
&+ \chi_{w,0}\Big(\partial_t(\varrho_0\boldsymbol{v}_{0,w}) - \mathrm{div}_y\,(\nu\nabla_y\boldsymbol{v}_{0,w}) - \nabla_y\,(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,w}) + \nabla_y p_{w,1} + \nabla_x p_w - \rho_w\boldsymbol{g}\Big)\\
&\quad + \chi_{w,0}\Big(\partial_t(\varrho_0\boldsymbol{v}_{0,I}) - \mathrm{div}_y\,(\nu\nabla_y\boldsymbol{v}_{0,I}) - \nabla_y\,(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,I}) + \mathrm{div}_y\,(\mathbb{T}_{c0})\Big)\\
&\quad + \chi_{I,0}\Big(\partial_t(\varrho_0\boldsymbol{v}_{0,w}) - \mathrm{div}_y\,(\nu\nabla_y\boldsymbol{v}_{0,w}) - \nabla_y\,(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,w})\Big)\\
&\quad + \chi_{I,0}\Big(\partial_t(\varrho_0\boldsymbol{v}_{0,a}) - \mathrm{div}_y\,(\nu\nabla_y\boldsymbol{v}_{0,a}) - \nabla_y\,(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,a}) - \tilde{\varrho}(x,c_0)\boldsymbol{g}\Big)\\
&\quad + \chi_{I,0}\Big(\partial_t(\varrho_0\boldsymbol{v}_{0,I}) - \mathrm{div}_y\,(\nu\nabla_y\boldsymbol{v}_{0,I}) - \nabla_y\,(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,I}) + \nabla_y p_I + \mathrm{div}_y\,(\mathbb{T}_{c0})\Big) = 0
\end{aligned}
$$

For the boundary conditions, we may proceed in the same way with $(8.5)_1$introducing the notation

$$
\mathfrak{F} := \varrho_0\left(\frac{\sigma_\Gamma}{\varrho_0}\Delta_{\tau\tau,yy}c_0 - \frac{f_\Gamma(c_0)}{\varrho_0}\right),
$$

and using (11.1) and (11.5):

$$
\begin{aligned}
(11.7)\quad & \chi_a\left[\left(\left(\nu\mathbb{D}_y\left(\boldsymbol{v}_{0,a}+\boldsymbol{v}_{0,I}\right) - \mathbb{T}_{c0}\right)\boldsymbol{n}_\Gamma\right)_\tau + \alpha_\Gamma\left(\boldsymbol{v}_{0,a}+\boldsymbol{v}_{0,I}\right)_\tau + \mathfrak{F}\,\nabla_{\tau,y}c_0\right]\\
&\quad + \chi_w\left[\left(\left(\nu\mathbb{D}_y\left(\boldsymbol{v}_{0,w}+\boldsymbol{v}_{0,I}\right) - \mathbb{T}_{c0}\right)\boldsymbol{n}_\Gamma\right)_\tau + \alpha_\Gamma\left(\boldsymbol{v}_{0,w}+\boldsymbol{v}_{0,I}\right)_\tau + \mathfrak{F}\,\nabla_{\tau,y}c_0\right]\\
&\quad \chi_a\left[\left(\left(\nu\mathbb{D}_y\left(\boldsymbol{v}_{0,a}+\boldsymbol{v}_{0,I}+\boldsymbol{v}_{0,w}\right) - \mathbb{T}_{c0}\right)\boldsymbol{n}_\Gamma\right)_\tau + \alpha_\Gamma\left(\boldsymbol{v}_{0,a}+\boldsymbol{v}_{0,I}+\boldsymbol{v}_{0,w}\right)_\tau + \mathfrak{F}\,\nabla_{\tau,y}c_0\right] = 0
\end{aligned}
$$

11.5. **The separated two-scale problems.** We rewrite equation (11.6) as

$$
\chi_a f_a + \chi_w f_w + \chi_I f_I = 0
$$

and boundary condition (11.7) as

$$
\chi_a B_a + \chi_w B_w + \chi_I B_I = 0
$$

with obvious implicit definition of $f_{a,w,I}$ and $B_{a,w,I}$. Then, due to the definition of χ_a, χ_w, χ_I, equation (11.6) can hold only if

$$
(11.8)\quad f_a = 0 \text{ on } \boldsymbol{Y}_1\backslash\left(\boldsymbol{Y}_w\cup\boldsymbol{Y}_I\right),\quad f_w = 0 \text{ on } \boldsymbol{Y}_1\backslash\left(\boldsymbol{Y}_a\cup\boldsymbol{Y}_I\right),\quad f_I = 0 \text{ on } \boldsymbol{Y}_1\backslash\left(\boldsymbol{Y}_w\cup\boldsymbol{Y}_a\right).
$$

The last condition is necessary for (11.6) to hold, but not sufficient. As a sufficient condition, we assume for simplicity that

$$
f_a = 0 \text{ on } \boldsymbol{Y}_a(x),\qquad f_w = 0 \text{ on } \boldsymbol{Y}_w(x)\qquad\text{and}\qquad f_I = 0 \text{ on } \boldsymbol{Y}_I(x),
$$

which in turn is much stronger than the necessary condition (11.8). Similarly, the boundary condition (11.7) is split up into

$$
B_a = 0 \text{ on } \Gamma\cap\partial\boldsymbol{Y}_a(x),\quad B_w = 0 \text{ on } \Gamma\cap\partial\boldsymbol{Y}_w(x)\quad\text{and}\quad B_I = 0 \text{ on } \Gamma\cap\partial\boldsymbol{Y}_I(x).
$$

Additionally, we have to account for

$$
\boldsymbol{v}_{0,a} = 0 \text{ on } \boldsymbol{Y}_1\backslash\boldsymbol{Y}_a(x),\quad \boldsymbol{v}_{0,w} = 0 \text{ on } \boldsymbol{Y}_1\backslash\boldsymbol{Y}_w(x)\quad\text{and}\quad \boldsymbol{v}_{0,I} = 0 \text{ on } \boldsymbol{Y}_1\backslash\boldsymbol{Y}_I(x).
$$

Then, the equation on $\boldsymbol{Y}_a(x)$ reads

$$
\begin{aligned}
(11.9a)\quad & \partial_t(\varrho_0\boldsymbol{v}_{0,a}) - \mathrm{div}_y\,(\nu\nabla_y\boldsymbol{v}_{0,a}) - \nabla_y\,(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,a}) + \nabla_y p_{a,1} + \nabla_x p_a - \rho_a\boldsymbol{g}\\
&\quad + \partial_t(\varrho_0\boldsymbol{v}_{0,I}) - \mathrm{div}_y\,(\nu\nabla_y\boldsymbol{v}_{0,I}) - \nabla_y\,(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,I}) + \mathrm{div}_y\,(\mathbb{T}_{c0}) = 0
\end{aligned}
$$

with the boundary conditions

$$\boldsymbol{v}_{0,a} = 0 \quad \text{on } \partial \boldsymbol{Y}_a(x)\backslash\Gamma \tag{11.9b}$$

$$\left((\nu \mathbb{D}_y\left(\boldsymbol{v}_{0,a}+\boldsymbol{v}_{0,I}\right)-\mathbb{T}_{c0})\,\boldsymbol{n}_\Gamma\right)_\tau + \alpha_\Gamma\left(\boldsymbol{v}_{0,a}+\boldsymbol{v}_{0,I}\right)_\tau + \mathfrak{F}\,\nabla_{\tau,y}c_0 = 0 \quad \text{on } \partial \boldsymbol{Y}_a(x)\cap\Gamma\,. \tag{11.9c}$$

The equation on $\boldsymbol{Y}_w(x)$ reads

$$\begin{aligned}\partial_t(\varrho_0\boldsymbol{v}_{0,w}) - \operatorname{div}_y\left(\nu\nabla_y\boldsymbol{v}_{0,w}\right) - \nabla_y\left(\lambda\operatorname{div}_y\boldsymbol{v}_{0,w}\right) + \nabla_y p_{w,1} + \nabla_x p_w - \rho_w\boldsymbol{g}\\ + \partial_t(\varrho_0\boldsymbol{v}_{0,I}) - \operatorname{div}_y\left(\nu\nabla_y\boldsymbol{v}_{0,I}\right) - \nabla_y\left(\lambda\operatorname{div}_y\boldsymbol{v}_{0,I}\right) + \operatorname{div}_y\left(\mathbb{T}_{c0}\right) = 0\end{aligned} \tag{11.10a}$$

with the boundary conditions

$$\boldsymbol{v}_{0,w} = 0 \quad \text{on } \partial \boldsymbol{Y}_w(x)\backslash\Gamma \tag{11.10b}$$

$$\left((\nu \mathbb{D}_y\left(\boldsymbol{v}_{0,w}+\boldsymbol{v}_{0,I}\right)-\mathbb{T}_{c0})\,\boldsymbol{n}_\Gamma\right)_\tau + \alpha_\Gamma\left(\boldsymbol{v}_{0,w}+\boldsymbol{v}_{0,I}\right)_\tau + \mathfrak{F}\,\nabla_{\tau,y}c_0 = 0 \quad \text{on } \partial \boldsymbol{Y}_w(x)\cap\Gamma\,. \tag{11.10c}$$

And finally, the equation on $\boldsymbol{Y}_I(x)$ reads

$$\begin{aligned}\partial_t(\varrho_0\boldsymbol{v}_{0,I}) - \operatorname{div}_y\left(\nu\nabla_y\boldsymbol{v}_{0,I}\right) - \nabla_y\left(\lambda\operatorname{div}_y\boldsymbol{v}_{0,I}\right) + \nabla_y p_I - \varrho_0\boldsymbol{g}\\ + \partial_t(\varrho_0\boldsymbol{v}_{0,w}) - \operatorname{div}_y\left(\nu\nabla_y\boldsymbol{v}_{0,w}\right) - \nabla_y\left(\lambda\operatorname{div}_y\boldsymbol{v}_{0,w}\right) + \operatorname{div}_y\left(\mathbb{T}_{c0}\right)\\ + \partial_t(\varrho_0\boldsymbol{v}_{0,a}) - \operatorname{div}_y\left(\nu\nabla_y\boldsymbol{v}_{0,a}\right) - \nabla_y\left(\lambda\operatorname{div}_y\boldsymbol{v}_{0,a}\right) = 0\end{aligned} \tag{11.11a}$$

with the boundary conditions

$$\boldsymbol{v}_{0,I} = 0 \quad \text{on } \partial \boldsymbol{Y}_I(x)\backslash\Gamma \tag{11.11b}$$

(11.11c)

$$\left((\nu \mathbb{D}_y\left(\boldsymbol{v}_{0,w}+\boldsymbol{v}_{0,a}+\boldsymbol{v}_{0,I}\right)-\mathbb{T}_{c0})\,\boldsymbol{n}_\Gamma\right)_\tau + \alpha_\Gamma\left(\boldsymbol{v}_{0,w}+\boldsymbol{v}_{0,a}+\boldsymbol{v}_{0,I}\right)_\tau + \mathfrak{F}\,\nabla_{\tau,y}c_0 = 0 \quad \text{on } \partial \boldsymbol{Y}_I(x)\cap\Gamma$$

11.6. **The stationary phase filed and stationary geometry problem.** We will now derive effective macroscopic permeability tensors using above splitting of (11.6). In a first approach, we consider stationary phase fields i.e. $\partial_t c_0 = 0$. Due to the definition of χ_I, we expect that

$$(1-\chi_I)\,\nabla_y c_0 \approx 0\,. \tag{11.12}$$

Thus, in $\boldsymbol{Y}_a(x)$ and $\boldsymbol{Y}_w(x)$, capillarity plays a minor role for the evolution of the velocity field. Also, since we are interested in the stationary geometry case, $\boldsymbol{v}_0$ is assumed to vanish in the transition zone, since otherwise the transition zone could move. The mathematical implication is

$$\boldsymbol{v}_{0,I} = \chi_I\boldsymbol{v}_0 \approx 0 \tag{11.13}$$

as well as

$$\boldsymbol{v}_{0,w} = \chi_w\boldsymbol{v}_0 \approx c_0\boldsymbol{v}_0 \quad \text{on } \boldsymbol{Y}_w \qquad \text{and} \qquad \boldsymbol{v}_{0,a} = \chi_a\boldsymbol{v}_0 \approx (1-c_0)\,\boldsymbol{v}_0 \quad \text{on } \boldsymbol{Y}_a\,. \tag{11.14}$$

Using these approximations in (11.9)-(11.11) yields:

$$\begin{aligned}-\operatorname{div}_y\left(\mu\nabla_y(\boldsymbol{v}_{0,a})\right) - \nabla_y\left(\lambda\operatorname{div}_y\left(c_0\boldsymbol{v}_{0,a}\right)\right) + \nabla_y p_{i,a} + \nabla_x p_a = \rho_a\boldsymbol{g} \quad \text{on } \boldsymbol{Y}_a\\ -\operatorname{div}_y\left(\mu\nabla_y(\boldsymbol{v}_{0,w})\right) - \nabla_y\left(\lambda\operatorname{div}_y\left(c_0\boldsymbol{v}_{0,w}\right)\right) + \nabla_y p_{i,w} + \nabla_x p_w = \rho_w\boldsymbol{g} \quad \text{on } \boldsymbol{Y}_w\end{aligned}$$

with the boundary conditions

$$\begin{aligned}\boldsymbol{v}_{0,a} = 0 \quad \text{on } \partial\boldsymbol{Y}_a\backslash\Gamma\\ \boldsymbol{v}_{0,w} = 0 \quad \text{on } \partial\boldsymbol{Y}_w\backslash\Gamma\end{aligned}$$

as well as

$$\begin{aligned}\left((\nu\mathbb{D}_y\left(\boldsymbol{v}_{0,a}\right))\,\boldsymbol{n}_\Gamma\right)_\tau + \alpha_\Gamma\left(\boldsymbol{v}_{0,a}\right)_\tau = 0 \quad \text{on } \Gamma\,,\\ \left((\nu\mathbb{D}_y\left(\boldsymbol{v}_{0,w}\right))\,\boldsymbol{n}_\Gamma\right)_\tau + \alpha_\Gamma\left(\boldsymbol{v}_{0,w}\right)_\tau = 0 \quad \text{on } \Gamma\,.\end{aligned}$$

Following section 3.1, we look for $\boldsymbol{u}_{i,a}$ and $\boldsymbol{u}_{i,w}$ satisfying

$$\begin{aligned} -\mathrm{div}_y\left(\mu\nabla_y\boldsymbol{u}_{i,a}\right)-\nabla_y\left(\lambda\mathrm{div}_y\,\boldsymbol{u}_{i,a}\right)+\nabla_y\Pi_{i,a}&=\boldsymbol{e}_i && \text{on } \boldsymbol{Y}_a(x)\\ \mathrm{div}_y\left(\varrho_0\boldsymbol{u}_{i,a}\right)&=0 && \text{on } \boldsymbol{Y}_a(x)\\ \boldsymbol{u}_{i,a}&\equiv 0 && \text{on } \left(\boldsymbol{Y}_w(x)\cup\boldsymbol{Y}_I(x)\right)\end{aligned} \tag{11.15}$$

and

$$\begin{aligned} -\mathrm{div}_y\left(\mu\nabla_y\boldsymbol{u}_{i,w}\right)-\nabla_y\left(\lambda\mathrm{div}_y\,\boldsymbol{u}_{i,w}\right)+\nabla_y\Pi_{i,w}&=\boldsymbol{e}_i && \text{on } \boldsymbol{Y}_w(x)\\ \mathrm{div}_y\left(\varrho_0\boldsymbol{u}_{i,w}\right)&=0 && \text{on } \boldsymbol{Y}_w(x)\\ \boldsymbol{u}_{i,w}&\equiv 0 && \text{on } \left(\boldsymbol{Y}_a(x)\cup\boldsymbol{Y}_I(x)\right)\end{aligned} \tag{11.16}$$

with the boundary conditions

$$\begin{aligned}\boldsymbol{u}_{i,a}&=0 \quad \text{on } \partial\boldsymbol{Y}_a\backslash\Gamma\\ \boldsymbol{u}_{i,w}&=0 \quad \text{on } \partial\boldsymbol{Y}_w\backslash\Gamma\end{aligned}$$

as well as

$$\begin{aligned}\left(\left(\nu\mathbb{D}_y\left(\boldsymbol{u}_{i,a}\right)\right)\boldsymbol{n}_\Gamma\right)_\tau+\alpha_\Gamma\left(\boldsymbol{u}_{i,a}\right)_\tau&=0 \quad \text{on } \Gamma\,,\\ \left(\left(\nu\mathbb{D}_y\left(\boldsymbol{u}_{i,w}\right)\right)\boldsymbol{n}_\Gamma\right)_\tau+\alpha_\Gamma\left(\boldsymbol{u}_{i,w}\right)_\tau&=0 \quad \text{on } \Gamma\,.\end{aligned}$$

Comparing with section 3.1, we see that

$$\begin{aligned}\left(1-c_0\right)\boldsymbol{v}_0\approx\boldsymbol{v}_{0,a}&:=\sum_i\boldsymbol{u}_{i,a}\left(\rho_a\boldsymbol{g}-\nabla_x p_a\right)_i\\ c_0\boldsymbol{v}_0\approx\boldsymbol{v}_{0,w}&:=\sum_i\boldsymbol{u}_{i,w}\left(\rho_w\boldsymbol{g}-\nabla_x p_w\right)_i\end{aligned}$$

which yields with (10.1b) and (10.2):

$$\begin{aligned}\bar{\boldsymbol{v}}_w&\approx\frac{1}{\bar{\varrho}_w}\sum\left[\left(\rho_A\boldsymbol{g}-\nabla_x p_w\right)_i(x)\right]\int_{\boldsymbol{Y}_1}\varrho_0 u_{i,w}(y)dy=A_w\left(\rho_A\boldsymbol{g}-\nabla_x p_w\right)\\ \bar{\boldsymbol{v}}_a&\approx\frac{1}{\bar{\varrho}_a}\sum\left[\left(\rho_W\boldsymbol{g}-\nabla_x p_a\right)_i(x)\right]\int_{\boldsymbol{Y}_1}\varrho_0 u_{i,a}(y)dy=A_a\left(\rho_W\boldsymbol{g}-\nabla_x p_a\right)\end{aligned}$$

with ρ_A and ρ_W taken from (11.2), where

$$\left(A_w\right)_{i,j}=a_{w,ij}=\frac{1}{\bar{\varrho}_w}\int_{\boldsymbol{Y}_1}\varrho_0 u_{i,w}(y)\cdot\boldsymbol{e}_j\,ds,\quad \left(A_a\right)_{i,j}=a_{a,ij}=\frac{1}{\bar{\varrho}_a}\int_{\boldsymbol{Y}_1}\varrho_0 u_{i,a}(y)\cdot\boldsymbol{e}_j\,ds\,.$$

Note that above formulas for A_w and A_a only have approximate character and are not to be taken for exact formulas. However, if the neglected terms are small, the above approximation is close to the true macroscopic behavior.

11.7. **The quasi stationary flow.** In contrast to 11.6, we will now consider the case that $\boldsymbol{v}_{0,I}$ is not negligible but still $\partial_t(\varrho_0\boldsymbol{v}_0)\approx 0$. This turns out to be the mathematically most complex case. Note once more, that we start from $\boldsymbol{v}_0$, $\boldsymbol{v}_{0,a}$, $\boldsymbol{v}_{0,w}$ and $\boldsymbol{v}_{0,I}$ and we seek for a representation of the macroscopic permeability tensor in terms of these microscopic quantities.

Having a look on the stationary problem of (11.9a)

$$\begin{aligned}-\mathrm{div}_y\left(\nu\nabla_y\boldsymbol{v}_{0,a}\right)-\nabla_y\left(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,a}\right)+\nabla_y p_{a,1}+\nabla_x p_a-\rho_a\boldsymbol{g}&\\ -\mathrm{div}_y\left(\nu\nabla_y\boldsymbol{v}_{0,I}\right)-\nabla_y\left(\lambda\mathrm{div}_y\,\boldsymbol{v}_{0,I}\right)+\mathrm{div}_y\left(\mathbb{T}_{c0}\right)&=0\end{aligned}$$

and comparing with section 3.1, one could get the idea that the resulting problems for $\boldsymbol{u}_{i,a}$ read

$$-\mathrm{div}_y\left(\mu\nabla_y\boldsymbol{u}_{i,a}\right)-\nabla_y\left(\lambda\mathrm{div}_y\,\boldsymbol{u}_{i,a}\right)+\nabla_y\Pi_i+G_i\boldsymbol{e}_i=\boldsymbol{e}_i\,, \tag{11.18}$$

where

$$G_i = \frac{1}{(\rho_a \boldsymbol{g} - \nabla_x p_a)_i} \left[-\mathrm{div}_y \left(\nu \nabla_y \boldsymbol{v}_{0,I} \right) - \nabla_y \left(\lambda \mathrm{div}_y \, \boldsymbol{v}_{0,I} \right) + \mathrm{div}_y \left(\mathbb{T}_{c0} \right) \right] \cdot \boldsymbol{e}_i \, .$$

However, note that we would run into serious troubles if $(\rho_a \boldsymbol{g} - \nabla_x p_a)_i = 0$, in particular, if the system approaches the case of zero air flux.

Thus, we seek for another ansatz: Remembering

$$\boldsymbol{v}_{0,a}/\chi_a = \boldsymbol{v}_0 = \boldsymbol{v}_{0,I}/\chi_I \quad \text{on } \boldsymbol{Y}_a(x) \cap \boldsymbol{Y}_I(x) \, ,$$

and using this formula in (11.9a), assuming $\nabla_y c_0(x,y) \approx 0$ on $\boldsymbol{Y}_a(x)$, leads to

$$-\mathrm{div}_y \left(\nu \nabla_y \left(\boldsymbol{v}_{0,a} \left(1 + \frac{\chi_I}{\chi_a} \right) \right) \right) - \nabla_y \left(\lambda \mathrm{div}_y \left(\boldsymbol{v}_{0,a} \left(1 + \frac{\chi_I}{\chi_a} \right) \right) \right) + \nabla_y p_{a,1} + \nabla_x p_a - \rho_a \boldsymbol{g} = 0 \, .$$

We perform a transformation of variables

$$\tilde{\boldsymbol{v}}_{0,a} := \boldsymbol{v}_{0,a} \left(1 + \frac{\chi_I}{\chi_a} \right) \tag{11.19}$$

and obtain

$$-\mathrm{div}_y \left(\nu \nabla_y \tilde{\boldsymbol{v}}_{0,a} \right) - \nabla_y \left(\lambda \mathrm{div}_y \, \tilde{\boldsymbol{v}}_{0,a} \right) + \nabla_y p_{a,1} + \nabla_x p_a - \rho_a \boldsymbol{g} = 0$$

together with the boundary condition (11.9b) replaced by

$$\tilde{\boldsymbol{v}}_{0,a} = \boldsymbol{v}_{0,I}(x, y_0) \quad \text{on } \partial \boldsymbol{Y}_a \backslash \Gamma \, . \tag{11.20}$$

Then, the cell problems on $\boldsymbol{Y}_a(x)$ read

$$\begin{aligned} -\mathrm{div}_y \left(\mu \nabla_y \boldsymbol{u}_{i,a} \right) & \\ -\nabla_y \left(\lambda \mathrm{div}_y \, \boldsymbol{u}_{i,a} \right) + \nabla_y \Pi_{i,a} = \boldsymbol{e}_i & \qquad \text{on } \boldsymbol{Y}_a(x) \\ \mathrm{div}_y \left[\varrho_0 \boldsymbol{u}_{i,a} \right] = 0 & \qquad \text{on } \boldsymbol{Y}_a(x) \end{aligned}$$

with the boundary conditions

$$\left(\left(\nu \mathbb{D}_y \boldsymbol{u}_{i,a} \right) \boldsymbol{n}_\Gamma \right)_\tau + \alpha_\Gamma \left(\boldsymbol{u}_{i,a} \right)_\tau = 0 \quad \text{on } \Gamma \tag{11.21}$$

and on $\partial \boldsymbol{Y}_a(x) \backslash \Gamma$ we prescribe in case $\boldsymbol{v}_{0,I}(x,y_0) \cdot \boldsymbol{e}_i \neq 0$:

$$\boldsymbol{u}_{i,a} = \begin{cases} \frac{\left(\boldsymbol{v}_{0,I}(x,y_0) \cdot \boldsymbol{e}_i \right)}{(\rho_a \boldsymbol{g} - \nabla_x p_a)_i} \boldsymbol{e}_i & \text{if } (\rho_a \boldsymbol{g} - \nabla_x p_a)_i \neq 0 \\ \lim_{\delta \to 0} \frac{\left(\boldsymbol{v}_{0,I}(x,y_0) \cdot \boldsymbol{e}_i \right)}{\delta} \boldsymbol{e}_i & \text{if } (\rho_a \boldsymbol{g} - \nabla_x p_a)_i = 0 \end{cases} \quad \text{on } \partial \boldsymbol{Y}_a \backslash \Gamma \, , \tag{11.22}$$

for a choice $\delta \ll \left| \boldsymbol{v}_{0,I}(x,y_0) \cdot \boldsymbol{e}_i \right|$.

The cell problem on $\boldsymbol{Y}_w(x)$ can be constructed similarly. The macroscopic velocity fields $\bar{\boldsymbol{v}}_w$ and $\bar{\boldsymbol{v}}_a$ defined in (10.1b) and (10.2) can then be obtained using

$$c_0 \boldsymbol{v}_0 \approx c_0 (\boldsymbol{v}_{0,w} + \boldsymbol{v}_{0,I}) \qquad \text{and} \qquad (1 - c_0) \, \boldsymbol{v}_0 \approx (1 - c_0) \, (\boldsymbol{v}_{0,a} + \boldsymbol{v}_{0,I}) \, .$$

Since $\boldsymbol{v}_{0,I}$ is restricted to the small transition zone, it has only minor impact on the macroscopic quantities $\bar{\boldsymbol{v}}_a$ and $\bar{\boldsymbol{v}}_w$. Therefore, we are not interested in cell solutions of (11.11). According to the above calculations, $\boldsymbol{v}_{0,w}$ and $\boldsymbol{v}_{0,a}$ are approximately given through

$$\begin{aligned} \boldsymbol{v}_{0,a} &= \sum_i \left(1 + \chi_I / \chi_a \right)^{-1} \boldsymbol{u}_{i,a} (\rho_A \boldsymbol{g} - \nabla_x p_a)_i \\ \boldsymbol{v}_{0,w} &= \sum_i \left(1 + \chi_I / \chi_w \right)^{-1} \boldsymbol{u}_{i,w} (\rho_W \boldsymbol{g} - \nabla_x p_w)_i \, . \end{aligned}$$

Then, the resulting constitutive equations for $\bar{\boldsymbol{v}}_w$ and $\bar{\boldsymbol{v}}_a$ read according to (10.1b) and (10.2):

$$\bar{\boldsymbol{v}}_w = \frac{1}{\bar{\varrho}_w}\int_{\boldsymbol{Y}} (1+\chi_I/\chi_w)^{-1}\left(\varrho_0 c_0 \sum_i \left[(\rho_W \boldsymbol{g} - \nabla_x p_w)_i\right]\boldsymbol{u}_{i,w} + \varrho_0 c_0 \boldsymbol{v}_{0,I}\right)$$
$$\bar{\boldsymbol{v}}_a = \frac{1}{\bar{\varrho}_a}\int_{\boldsymbol{Y}} (1+\chi_I/\chi_a)^{-1}\left(\varrho_0 (1-c_0) \sum_i \left[(\rho_A \boldsymbol{g} - \nabla_x p_a)_i\right]\boldsymbol{u}_{i,a} + \varrho_0 (1-c_0) \boldsymbol{v}_{0,I}\right).$$

Since the transition zone is thin, even on the pore scale, it can be assumed that

$$\int_{\boldsymbol{Y}} \left|\varrho_0 \boldsymbol{v}_{0,I}\right| \approx 0$$

and the resulting equations for $\bar{\boldsymbol{v}}_a$ and $\bar{\boldsymbol{v}}_w$ read

$$\bar{\boldsymbol{v}}_w = A_w\left(\rho_W \boldsymbol{g} - \nabla_x p_w\right)$$
$$\bar{\boldsymbol{v}}_a = A_a\left(\rho_A \boldsymbol{g} - \nabla_x p_a\right).$$

with

$$(A_{w,ij})_{ij} = \frac{1}{\bar{\varrho}_w}\int_{\boldsymbol{Y}} (1+\chi_I/\chi_w)^{-1}\left(c_0\varrho_0 \boldsymbol{u}_{i,w}\cdot\boldsymbol{e}_j\right) \quad \text{and} \quad (A_{a,ij})_{ij} = \frac{1}{\bar{\varrho}_a}\int_{\boldsymbol{Y}} (1+\chi_I/\chi_a)^{-1}\left((1-c_0)\varrho_0 \boldsymbol{u}_{i,a}\cdot\boldsymbol{e}_j\right).$$

Even though the moving of the microscopic interface seems to have no influence on the macroscopic equations, note that this is not the case: due to the microscopic boundary conditions for $\boldsymbol{u}_{i,a}$ and $\boldsymbol{u}_{i,w}$, these functions strongly depend on the velocity field $\boldsymbol{v}_{0,I}$ and therefore also the permeabilities.

11.8. **The dynamic case.** In case $\partial_t(\varrho_0 \boldsymbol{v}_0) \approx 0$ is no longer justified, the above calculations in 11.7 could be repeated with $(\rho_A \boldsymbol{g} - \nabla_x p_a)$ and $(\rho_W \boldsymbol{g} - \nabla_x p_w)$, replaced by $\partial_t(\rho_A \boldsymbol{g} - \nabla_x p_a)$ and $\partial_t(\rho_W \boldsymbol{g} - \nabla_x p_w)$. Using (11.19) and (11.20), the function $\boldsymbol{u}_{i,a}$ has to solve the non-stationary problem

$$\begin{aligned}
\partial_t\left(\rho_a\left(\boldsymbol{u}_{i,a}\right)\right) - \operatorname{div}_y\left(\mu\nabla_y\left(\boldsymbol{u}_{i,a}\right)\right) & \\
-\nabla_y\left(\lambda \operatorname{div}_y\left(\boldsymbol{u}_{i,a}\right)\right) + \nabla_y \Pi_{i,a} = \boldsymbol{e}_i & \qquad \text{on } \boldsymbol{Y}_a(x) \\
\operatorname{div}_y\left[\varrho_0 \boldsymbol{u}_{i,a}\right] = 0 & \qquad \text{on } \boldsymbol{Y}_a(x) \\
\boldsymbol{u}_{i,a}(t=0,\cdot) = 0 & \qquad \text{on } \boldsymbol{Y}_1
\end{aligned}$$

with boundary conditions (11.21) and (11.22). Additionally, we would need a function $\hat{\boldsymbol{v}}$ as a solution of

$$\begin{aligned}
\partial_t\left(\varrho_0 \hat{\boldsymbol{v}}\right) - \operatorname{div}_y\left(\nu\nabla_y \hat{\boldsymbol{v}}\right) + \nabla_y p_1 = 0 & \qquad \text{on } (0,t)\times\boldsymbol{Y}_1 \\
\operatorname{div}_y\left(\varrho_0 \hat{\boldsymbol{v}}\right) = \partial_t \varrho_0 & \qquad \text{on } (0,t)\times\boldsymbol{Y}_1 \\
\hat{\boldsymbol{v}}(0,\cdot) = \hat{\boldsymbol{v}}_0(\cdot) & \qquad \text{on } \boldsymbol{Y}_1
\end{aligned}$$

where $\hat{\boldsymbol{v}}_0$ is the initial value of $\boldsymbol{v}_0$:

$$\boldsymbol{v}_0(t=0,\cdot) = \hat{\boldsymbol{v}}_0(\cdot).$$

Then, following section 3 and the above calculations, we obtain

$$\bar{\boldsymbol{v}}_w \approx \frac{1}{\bar{\varrho}_w}\int_{\boldsymbol{Y}}\left(c_0\varrho_0\hat{\boldsymbol{v}} + c_0\varrho_0\int_0^t \sum\left[\partial_t\left(\rho_W\boldsymbol{g} - \nabla_x p_w\right)_i(s,x)\right]\left(1+\frac{\chi_I}{\chi_w}\right)^{-1}\boldsymbol{u}_{i,w}(t-s,y)ds\right).$$
$$\bar{\boldsymbol{v}}_a \approx \frac{1}{\bar{\varrho}_a}\int_{\boldsymbol{Y}}\left((1-c_0)\varrho_0\hat{\boldsymbol{v}} + (1-c_0)\varrho_0\int_0^t \sum\left[\partial_t\left(\rho_A\boldsymbol{g} - \nabla_x p_a\right)_i(s,x)\right]\left(1+\frac{\chi_I}{\chi_a}\right)^{-1}\boldsymbol{u}_{i,a}(t-s,y)ds\right).$$

12. Capillary Pressure and Richard's Equation

If the air is assumed to move freely in the porous medium and is always at atmospheric pressure, it is often possible to neglect air transport and to focus on water transport only. Water transport is then described by the velocity field

$$\bar{\boldsymbol{v}}_w = A_c(\rho_W \boldsymbol{g} - \nabla p_c)\,, \tag{12.1}$$

with

$$p_c := p_w - p_a\,.$$

Equation (12.1) is called Buckimham-Darcy law and p_c is known as capillary pressure. The Buckingham-Darcy law inserted into (10.3a) yields the so called Richards equation[40]:

$$\partial_t \bar{\varrho}_w + \varepsilon \mathrm{div}_x\left(\bar{\varrho}_w A_c(\rho_W \boldsymbol{g} - \nabla p_c)\right) = 0\,.$$

This system usually is complemented by a relation $p_c = \tilde{p}_c(\bar{\varrho}_w)$. The author agrees with Hilfer [25], who states that capillary pressure should be an outcome of theory, not an input, appearing only in special cases. We assume that such a case is given by only slowly varying microscopic geometry in the Richards setting. However, the question remains how the capillary pressure p_c can be calculated from above two-scale model.

Classically, p_c is assumed to be related to the pressure jump across the microscopic interfaces. Since the phase field model does not contain interfaces but only a transition zone, there is also no pressure jump but only a pressure gradient.

For any pressure field p and any two points $x_1, x_2 \in \mathbb{R}^3$, the pressure difference between these two points is given by

$$p(x_1) - p(x_2) = \int_0^1 \nabla p(x_1 + s(x_2 - x_1)) \cdot (x_2 - x_1)\, ds\,.$$

Comparing with above approach in section 11, we get the approximation

$$p_c(x) \approx \left(\int_{\boldsymbol{Y}_I(x)} |\nabla_y p_{c,0}|\right) / \left(\int_{\boldsymbol{Y}_I(x)}\right)\,.$$

Here, $p_{c,0}$ is the mean normal stress across the transition zone:

$$p_{c,0} = \varepsilon p_0 + \frac{1}{3}\sigma \mathrm{tr}\left(\nabla_y c_0 \otimes \nabla_y c_0\right)\,,$$

where one should be aware of the fact, that p_0 itself depends on $\nabla_y c_0$.

13. Outlook

We discussed the homogenization of porous media twophase flow combining the assumption of maximum rate of entropy production with formal asymptotic expansion. The calculations are rather simple and can be easily performed, modified and adapted to much more general situations.

The approach as well as the resulting model are new and look different from any previously published model. At a second glance, under some assumption on the evolution of geometry, one can show that the model leads to the expected macroscopic behavior as well as to the classical macroscopic models. Thus, the two-scale model is a true generalization of existing macroscopic models.

The author believes that theoretical considerations on the basis of the above methods might help to find new and efficient algorithms for numerical simulations. Such simulations may complement and enrich existing approaches as they allow for implementation and quantification of interactions between micro and macro scale.

As the assumption of maximum rate of entropy production can be formulated on a very general level, further development can be expected for multiphase systems (see also Heida [19]), to erosion

or to swelling. However, note that the entropy method used in this paper is not yet at a level of generality to treat such problems and some effort also has to be put onto this subject.

Appendix A. Asymptotic expansion of the balance of entropy

In order to obtain two-scale entropy balance equations, we use a Taylor expansion in

$$\begin{aligned}\frac{1}{\vartheta^\varepsilon} &= \frac{1}{\vartheta_0} - \frac{1}{\vartheta_0^2}\left(\varepsilon\vartheta_1 + \varepsilon^2\vartheta_2\right) + \frac{1}{\vartheta_0^3}\left(\varepsilon\vartheta_1 + \varepsilon^2\vartheta_2\right)^2 + \mathcal{O}(\varepsilon^3)\\ \boldsymbol{q}^\varepsilon &= \varepsilon^{-1}\boldsymbol{q}_{-1} + \boldsymbol{q}_0 + \varepsilon\boldsymbol{q}_1\end{aligned}$$

with

$$\tilde{\boldsymbol{q}}^\varepsilon := \frac{\boldsymbol{q}^\varepsilon}{\vartheta^\varepsilon} = \varepsilon^{-1}\frac{\boldsymbol{q}_{-1}}{\vartheta_0} + \frac{\boldsymbol{q}_0}{\vartheta_0} + \frac{\boldsymbol{q}_{-1}}{\vartheta_0^2}\vartheta_1 + \varepsilon\left(\frac{\boldsymbol{q}_1}{\vartheta_0} - \frac{\boldsymbol{q}_0}{\vartheta_0^2}\vartheta_1 + \frac{\boldsymbol{q}_{-1}}{\vartheta_0^3}\vartheta_1^2\right) + \mathcal{O}(\varepsilon^2)$$

and define

$$\tilde{\boldsymbol{q}}_{-1} := \frac{\boldsymbol{q}_{-1}}{\vartheta_0}, \quad \tilde{\boldsymbol{q}}_0 := \frac{\boldsymbol{q}_0}{\vartheta_0} + \frac{\boldsymbol{q}_{-1}}{\vartheta_0^2}\vartheta_1 \quad \tilde{\boldsymbol{q}}_1 := \left(\frac{\boldsymbol{q}_1}{\vartheta_0} - \frac{\boldsymbol{q}_0}{\vartheta_0^2}\vartheta_1 + \frac{\boldsymbol{q}_{-1}}{\vartheta_0^3}\vartheta_1^2\right).$$

Then, one obtains

$$\partial_t\left(\varrho_0\eta_0\right) + \mathrm{div}_y\left(\varrho_0\eta_0\boldsymbol{v}_0\right) + \mathrm{div}_x\left(\varrho_0\eta_0\boldsymbol{v}_0\right) + \mathrm{div}_x\left(\tilde{\boldsymbol{q}}_0\right) + \mathrm{div}_y\left(\tilde{\boldsymbol{q}}_1\right) = \frac{\xi_0}{\vartheta_0},$$

with

$$\begin{aligned}\xi_0 &= \left(\mathbb{T} + \mathbb{T}_{c,0}\right)\cdot\mathbb{D}_y\boldsymbol{v}_0 + \tilde{\boldsymbol{q}}_0\cdot\left(\nabla_x\vartheta_0 + \nabla_y\vartheta_1\right) + \tilde{\boldsymbol{q}}_1\cdot\nabla_y\vartheta_0\\ &\quad + \tilde{\boldsymbol{q}}_{-1}\cdot\left(\nabla_x\vartheta_1 + \nabla_y\vartheta_2\right) + p_0\mathrm{div}_y\,\boldsymbol{v}_0 - \boldsymbol{j}_{1,0}\cdot\nabla_y\left(\mu_c + \mu\right),\\ \boldsymbol{q}_0 &= \kappa_1\nabla_x\vartheta_0 + \kappa_1\nabla_y\vartheta_1 + \kappa_{1,1}\nabla_y\vartheta_0,\\ \boldsymbol{q}_1 &= \kappa_1\nabla_x\vartheta_1 + \kappa_1\nabla_y\vartheta_2 + \kappa_{1,1}\nabla_y\vartheta_1 + \kappa_{1,1}\nabla_x\vartheta_0 + \kappa_{1,2}\nabla_y\vartheta_0\\ \boldsymbol{q}_{-1} &= \kappa_1\nabla_y\vartheta_0\end{aligned} \tag{A.1}$$

and we find additionally

$$\mathrm{div}_y\left(\tilde{\boldsymbol{q}}_{-1}\right) = \tilde{\boldsymbol{q}}_{-1}\cdot\nabla_y\vartheta_0 \tag{A.2a}$$

$$\mathrm{div}_y\left(\tilde{\boldsymbol{q}}_0\right) + \mathrm{div}_x\left(\tilde{\boldsymbol{q}}_{-1}\right) = \tilde{\boldsymbol{q}}_{-1}\cdot\left(\nabla_x\vartheta_0 + \nabla_y\vartheta_1\right) + \tilde{\boldsymbol{q}}_0\cdot\left(\nabla_y\vartheta_0\right). \tag{A.2b}$$

On $\boldsymbol{Q}\times\boldsymbol{Y}_2$, we find with the notations

$$\tilde{\boldsymbol{q}}_2^\varepsilon := \frac{\boldsymbol{q}^\varepsilon}{\vartheta^\varepsilon} = \varepsilon^{-1}\frac{\boldsymbol{q}_{2,-1}}{\vartheta_0} + \frac{\boldsymbol{q}_{2,0}}{\vartheta_0} + \frac{\boldsymbol{q}_{2,-1}}{\vartheta_0^2}\vartheta_1 + \varepsilon\left(\frac{\boldsymbol{q}_{2,1}}{\vartheta_0} - \frac{\boldsymbol{q}_{2,0}}{\vartheta_0^2}\vartheta_1 + \frac{\boldsymbol{q}_{2,-1}}{\vartheta_0^3}\vartheta_1^2\right) + \mathcal{O}(\varepsilon^2),$$

$$\tilde{\boldsymbol{q}}_{2,-1} := \frac{\boldsymbol{q}_{2,-1}}{\vartheta_0}, \quad \tilde{\boldsymbol{q}}_{2,0} := \frac{\boldsymbol{q}_{2,0}}{\vartheta_0} + \frac{\boldsymbol{q}_{2,-1}}{\vartheta_0^2}\vartheta_1 \quad \tilde{\boldsymbol{q}}_{2,1} := \left(\frac{\boldsymbol{q}_{2,1}}{\vartheta_0} - \frac{\boldsymbol{q}_{2,0}}{\vartheta_0^2}\vartheta_1 + \frac{\boldsymbol{q}_{2,-1}}{\vartheta_0^3}\vartheta_1^2\right)$$

the local balance of entropy

$$\partial_t\left(\varrho_0\eta_{2,0}\right) + \mathrm{div}_y\left(\varrho_0\eta_{2,0}\boldsymbol{v}_0\right) + \mathrm{div}_x\left(\varrho_0\eta_{2,0}\boldsymbol{v}_0\right) + \mathrm{div}_x\left(\tilde{\boldsymbol{q}}_0\right) + \mathrm{div}_y\left(\tilde{\boldsymbol{q}}_1\right) = \frac{\xi_{2,0}}{\vartheta_0},$$

where the coefficients are given in a similar way to (A.1), except for the missing terms due to $\boldsymbol{v} = 0$ and $\varrho = const$, and we find additionally

$$\mathrm{div}_y\left(\tilde{\boldsymbol{q}}_{2,-1}\right) = \tilde{\boldsymbol{q}}_{2,-1}\cdot\nabla_y\vartheta_0 \tag{A.3a}$$

$$\mathrm{div}_y\left(\tilde{\boldsymbol{q}}_{2,0}\right) + \mathrm{div}_x\left(\tilde{\boldsymbol{q}}_{2,-1}\right) = \tilde{\boldsymbol{q}}_{2,-1}\cdot\left(\nabla_x\vartheta_0 + \nabla_y\vartheta_1\right) + \tilde{\boldsymbol{q}}_{2,0}\cdot\left(\nabla_y\vartheta_0\right). \tag{A.3b}$$

On $\boldsymbol{Q}\times\Gamma$ holds:

$$\begin{aligned}\partial_t\eta_{\Gamma,0} &= \frac{1}{\vartheta_0}\left(\boldsymbol{q}_{\Gamma,0}\cdot\frac{\nabla_{\tau,y}\vartheta_0}{\vartheta_0} + \overset{\oplus}{E} - \boldsymbol{v}_{0,\tau}\cdot\left[-\varrho_0\mu_{\Gamma,2}\nabla_{\tau,y}c_0\right] - \mu_{\Gamma,2}\overset{\oplus}{c}\right) + \mathrm{div}_{\tau,y}\left(\frac{\boldsymbol{q}_{\Gamma,0}}{\vartheta_0}\right)\\ \boldsymbol{q}_{\Gamma,0} &= \kappa_{\Gamma_0}\nabla_{\tau,y}\vartheta_0,\end{aligned}$$

Note that $\nabla_{\tau,y}\vartheta_0 = 0$ since $\nabla_y \vartheta_0 = 0$.

Interestingly, the lower order balance of entropy equations (A.2) and (A.3) are identical with (10.4).

Appendix B. Formal error estimates

We will compare formal error estimates for vanishing and non-vanishing macroscopic convection in order to give more justification for the approach in section 8.

B.1. **Vanishing macroscopic convection.** We consider the system

$$\begin{aligned} \partial_t \varrho^\varepsilon + \varepsilon \mathrm{div}\,(\varrho^\varepsilon \boldsymbol{v}_0^\varepsilon) &= 0 \\ \partial_t(\varrho^\varepsilon c^\varepsilon) + \varepsilon \mathrm{div}\,(\varrho^\varepsilon c^\varepsilon \boldsymbol{v}_0^\varepsilon) - \varepsilon^2 \Delta c^\varepsilon &= 0 \end{aligned} \tag{B.1}$$

where $\boldsymbol{v}_0^\varepsilon(t,x) := \boldsymbol{v}_0(t,x,\frac{x}{\varepsilon})$ with a given $\boldsymbol{v}_0$ with bounded divergence:

$$\|\mathrm{div}_x\, \boldsymbol{v}_0\|_{L^\infty} + \|\mathrm{div}_y\, \boldsymbol{v}_0\|_{L^\infty} \le C_{\boldsymbol{v}} < \infty$$

and zero flux boundary condition

$$\begin{aligned} \boldsymbol{v}_0 \cdot \nu &= 0 \quad \text{on } \partial \boldsymbol{Q} \times \boldsymbol{Y} \\ \boldsymbol{v}_0 \cdot \boldsymbol{n}_\Gamma &= 0 \quad \text{on } \boldsymbol{Q} \times \Gamma\,. \end{aligned}$$

The homogenized system for the first order approximations ϱ_0 and c_0 reads

$$\begin{aligned} \partial_t \varrho_0 + \mathrm{div}_y\,(\varrho_0 \boldsymbol{v}_0) &= 0 \\ \partial_t(\varrho_0 c_0) + \mathrm{div}_y\,(\varrho_0 c_0 \boldsymbol{v}_0) - \Delta_{yy} c_0 &= 0 \end{aligned}$$

We use

$$\nabla = \nabla_x + \frac{1}{\varepsilon}\nabla_y \quad \text{and} \quad \mathrm{div} = \mathrm{div}_x + \frac{1}{\varepsilon}\mathrm{div}_y$$

and find for $\varrho_0^\varepsilon(x) := \varrho_0(x,\frac{x}{\varepsilon})$ and $c_0^\varepsilon(x) := c_0(x,\frac{x}{\varepsilon})$:

$$\begin{aligned} \partial_t \varrho_0^\varepsilon + (\varepsilon \mathrm{div} - \varepsilon \mathrm{div}_x)\,(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon) &= 0 \\ \partial_t(\varrho_0^\varepsilon c_0^\varepsilon) + (\varepsilon \mathrm{div} - \varepsilon \mathrm{div}_x)\,(\varrho_0^\varepsilon c_0^\varepsilon \boldsymbol{v}_0^\varepsilon) - (\varepsilon \mathrm{div} - \varepsilon \mathrm{div}_x)\,(\varepsilon\,(\nabla - \nabla_x)\, c_0^\varepsilon) &= 0\,. \end{aligned} \tag{B.2}$$

Assuming that all functions posses enough regularity the difference of $(\mathrm{B.1})_1$ and $(\mathrm{B.2})_1$ reads:

$$\partial_t(\varrho_0^\varepsilon - \varrho^\varepsilon) + \varepsilon \mathrm{div}\,\left((\varrho_0^\varepsilon - \varrho^\varepsilon)\,\boldsymbol{v}_0^\varepsilon\right) = \varepsilon \mathrm{div}_x\,(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon)$$

which yields by testing with $(\varrho_0^\varepsilon - \varrho^\varepsilon)$ and partial integration

$$\frac{1}{2}\int_{\boldsymbol{Q}_1^\varepsilon} \partial_t\left((\varrho_0^\varepsilon - \varrho^\varepsilon)^2\right) + \varepsilon \int_{\boldsymbol{Q}_1^\varepsilon} \frac{1}{2}\boldsymbol{v}_0^\varepsilon \cdot \nabla\left((\varrho_0^\varepsilon - \varrho^\varepsilon)^2\right) = \varepsilon \int_{\boldsymbol{Q}_1^\varepsilon} \mathrm{div}_x\,(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon)\,(\varrho_0^\varepsilon - \varrho^\varepsilon)$$

and finally

$$\frac{d}{dt}\int_{\boldsymbol{Q}_1^\varepsilon} (\varrho_0^\varepsilon - \varrho^\varepsilon)^2 + \int_{\boldsymbol{Q}_1^\varepsilon} (\varrho_0^\varepsilon - \varrho^\varepsilon)^2 \varepsilon \mathrm{div}\,\boldsymbol{v}_0^\varepsilon \le \varepsilon^2 \left\|\mathrm{div}_x\,(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon)\right\|^2_{L^2(\boldsymbol{Q}_1^\varepsilon)} + \left\|\varrho_0^\varepsilon - \varrho^\varepsilon\right\|^2_{L^2(\boldsymbol{Q}_1^\varepsilon)}\,.$$

The last equation can be brought into the form

$$\frac{d}{dt}\int_{\boldsymbol{Q}_1^\varepsilon} (\varrho_0^\varepsilon - \varrho^\varepsilon)^2 \le \varepsilon^2 C_{\boldsymbol{v}}^2 + (1 + \varepsilon C_{\boldsymbol{v}})\left\|\varrho_0^\varepsilon - \varrho^\varepsilon\right\|^2_{L^2(\boldsymbol{Q}_1^\varepsilon)}$$

such that Gronwall's inequality yields

$$\left\|\varrho_0^\varepsilon(t) - \varrho^\varepsilon(t)\right\|^2_{L^2(\boldsymbol{Q}_1^\varepsilon)} \le \varepsilon^2 C_{\boldsymbol{v}}^2 t + \left\|\varrho_0^\varepsilon(0) - \varrho^\varepsilon(0)\right\|^2_{L^2(\boldsymbol{Q}_1^\varepsilon)} \exp\left((1 + \varepsilon C_{\boldsymbol{v}})\, t\right) \tag{B.3}$$

Now, build the difference of equations $(\mathrm{B.1})_2$ and $(\mathrm{B.2})_2$ to obtain

$$\begin{aligned} &\varrho_0^\varepsilon \partial_t\,(c_0^\varepsilon - c^\varepsilon) + (\varrho_0^\varepsilon - \varrho^\varepsilon)\,\partial_t c^\varepsilon + \varepsilon \varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon \nabla\,(c_0^\varepsilon - c^\varepsilon) + \varepsilon\,(\varrho_0^\varepsilon - \varrho^\varepsilon)\,\boldsymbol{v}_0^\varepsilon \nabla c^\varepsilon \\ &\qquad - \varepsilon \varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon \nabla_x c_0^\varepsilon - \varepsilon^2 \Delta\,(c_0^\varepsilon - c^\varepsilon) - \varepsilon^2 \mathrm{div}_x\,\nabla c_0^\varepsilon - \varepsilon^2 \mathrm{div}\,\nabla_x c_0^\varepsilon - \varepsilon^2 \Delta_{xx} c_0^\varepsilon = 0 \end{aligned}$$

which yields after testing with $(c_0^\varepsilon - c^\varepsilon)$:

$$\frac{1}{2}\frac{d}{dt}\int_{\boldsymbol{Q}_1^\varepsilon} \varrho_0^\varepsilon \left(c_0^\varepsilon - c^\varepsilon\right)^2 - \int_{\boldsymbol{Q}_1^\varepsilon} \varepsilon \mathrm{div}\left(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon\right)\left(c_0^\varepsilon - c^\varepsilon\right)^2 + \int_{\boldsymbol{Q}_1^\varepsilon} \left(\varrho_0^\varepsilon - \varrho^\varepsilon\right)\left[\partial_t c^\varepsilon + \varepsilon \boldsymbol{v}_0^\varepsilon \cdot \nabla c^\varepsilon\right]\left(c_0^\varepsilon - c^\varepsilon\right) - \int_{\boldsymbol{Q}_1^\varepsilon} \varepsilon \varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon \cdot \nabla_x c_0^\varepsilon \left(c_0^\varepsilon - c^\varepsilon\right) + \int_{\boldsymbol{Q}_1^\varepsilon} \varepsilon^2 \left|\nabla\left(c_0^\varepsilon - c^\varepsilon\right)\right|^2 + 2\int_{\boldsymbol{Q}_1^\varepsilon} \varepsilon^2 \nabla_x c_0^\varepsilon \cdot \nabla\left(c_0^\varepsilon - c^\varepsilon\right) - \int_{\boldsymbol{Q}_1^\varepsilon} \varepsilon^2 \Delta_{xx} c_0^\varepsilon \cdot \left(c_0^\varepsilon - c^\varepsilon\right) = 0\,.$$

The best estimates can be obtained if it is assumed that ϱ_0, $\boldsymbol{v}_0$, $\nabla_x c_0$ and $\Delta_{xx} c_0$ are essentially bounded. In this case, using $(\mathrm{B}.1)_2$, Hölder's inequality and $\|c_0^\varepsilon - c^\varepsilon\|_{L^2(\boldsymbol{Q}_1^\varepsilon)} \leq$, we get

$$\frac{1}{2}\frac{d}{dt}\int_{\boldsymbol{Q}_1^\varepsilon} \varrho_0^\varepsilon \left(c_0^\varepsilon - c^\varepsilon\right)^2 + \frac{1}{2}\int_{\boldsymbol{Q}_1^\varepsilon} \varepsilon^2 \left|\nabla\left(c_0^\varepsilon - c^\varepsilon\right)\right|^2 \leq \int_{\boldsymbol{Q}_1^\varepsilon} \varrho_0^\varepsilon \left(c_0^\varepsilon - c^\varepsilon\right)^2 + C_1 + C_2 \int_{\boldsymbol{Q}_1^\varepsilon} \left(c_0^\varepsilon - c^\varepsilon\right)^2 \tag{B.4a}$$

with

$$C_1 = \varepsilon^2 \int_{\boldsymbol{Q}_1^\varepsilon} \left(\left|\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon \cdot \nabla_x c_0^\varepsilon\right|^2 + 2\left|\nabla_x c_0^\varepsilon\right|^2 + \left(\varepsilon \Delta_{xx} c_0^\varepsilon\right)^2 + \left(\frac{\varepsilon}{\varrho^\varepsilon}\Delta c^\varepsilon \left(\varrho_0^\varepsilon - \varrho^\varepsilon\right)\right)^2 \right) \tag{B.4b}$$

$$C_2 = 1 + \left|\varepsilon \mathrm{div}_x\left(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon\right)\right| + \left|\mathrm{div}_y\left(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon\right)\right|\,. \tag{B.4c}$$

Since $\varepsilon^2 \Delta c^\varepsilon$ and $(\varrho_0^\varepsilon - \varrho^\varepsilon)$ is of order $\mathcal{O}(\varepsilon)$ (due to (B.3)), C_1 formally is of order $\mathcal{O}(\varepsilon)$: $C_1 = \mathcal{O}(\varepsilon)$ and $C_2 = \mathcal{O}(1)$.

B.2. **Macroscopic convection in the limit equations.** We consider the same system of equations but keep a convective term $\varepsilon^* \mathrm{div}_x\left(\varrho_0 \boldsymbol{v}_0\right)$ in the limit equations. The approximating system for the first order approximations ϱ_0 and c_0 then reads

$$\partial_t \varrho_0 + \varepsilon^* \mathrm{div}_x\left(\varrho_0 \boldsymbol{v}_0\right) + \mathrm{div}_y\left(\varrho_0 \boldsymbol{v}_0\right) = 0$$
$$\partial_t(\varrho_0 c_0) + \varepsilon^* \mathrm{div}_x\left(\varrho_0 c_0 \boldsymbol{v}_0\right) + \mathrm{div}_y\left(\varrho_0 c_0 \boldsymbol{v}_0\right) - \Delta_{yy} c_0 = 0$$

For suitable boundary conditions, we find

$$\partial_t \varrho_0^\varepsilon + \left(\varepsilon \mathrm{div}\, - \varepsilon \mathrm{div}_x\right)\left(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon\right) = 0$$
$$\partial_t(\varrho_0^\varepsilon c_0^\varepsilon) + \varepsilon^* \mathrm{div}_x\left(\varrho_0 c_0 \boldsymbol{v}_0\right) + \left(\varepsilon \mathrm{div}\, - \varepsilon \mathrm{div}_x\right)\left(\varrho_0^\varepsilon c_0^\varepsilon \boldsymbol{v}_0^\varepsilon\right) - \left(\varepsilon \mathrm{div}\, - \varepsilon \mathrm{div}_x\right)\left(\varepsilon\left(\nabla - \nabla_x\right) c_0^\varepsilon\right) = 0$$

We assume that all functions possess enough regularity and start by comparing the convective equations:

$$\partial_t(\varrho_0^\varepsilon - \varrho^\varepsilon) + \varepsilon \mathrm{div}\,\left(\left(\varrho_0^\varepsilon - \varrho^\varepsilon\right)\boldsymbol{v}_0^\varepsilon\right) = \left(\varepsilon - \varepsilon^*\right)\mathrm{div}_x\,\left(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon\right)$$

which yields by testing with $(\varrho_0^\varepsilon - \varrho^\varepsilon)$ and partial integration

$$\frac{d}{dt}\int (\varrho_0^\varepsilon - \varrho^\varepsilon)^2 + \int (\varrho_0^\varepsilon - \varrho^\varepsilon)^2 \varepsilon \mathrm{div}\, \boldsymbol{v}_0^\varepsilon \leq \left(\varepsilon - \varepsilon^*\right)^2 \left\|\mathrm{div}_x\,\left(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon\right)\right\|_{L^2}^2 + \left\|\varrho_0^\varepsilon - \varrho^\varepsilon\right\|_{L^2}^2$$

or

$$\frac{d}{dt}\int (\varrho_0^\varepsilon - \varrho^\varepsilon)^2 \leq \left(\varepsilon - \varepsilon^*\right)^2 \left\|\mathrm{div}_x\,\left(\varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon\right)\right\|_{L^2}^2 + \left(1 + \left|\varepsilon \mathrm{div}\, \boldsymbol{v}_0^\varepsilon\right|\right)\left\|\varrho_0^\varepsilon - \varrho^\varepsilon\right\|_{L^2}^2$$

which is for $\varepsilon = \varepsilon^*$ the optimal estimate:

$$\left\|\varrho_0^\varepsilon(t) - \varrho^\varepsilon(t)\right\|_{L^2(\boldsymbol{Q}_1^\varepsilon)}^2 \leq \left\|\varrho_0^\varepsilon(0) - \varrho^\varepsilon(0)\right\|_{L^2(\boldsymbol{Q}_1^\varepsilon)}^2 \exp\left(\left(1 + \varepsilon C_{\boldsymbol{v}}\right) t\right) = 0\,,$$

if $\varrho_0^\varepsilon(0) - \varrho^\varepsilon(0) = 0$.

Now, build the difference of the diffusion equations to obtain

$$\varrho_0^\varepsilon \partial_t \left(c_0^\varepsilon - c^\varepsilon\right) + \left(\varrho_0^\varepsilon - \varrho^\varepsilon\right) \partial_t c^\varepsilon + \varepsilon \varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon \nabla \left(c_0^\varepsilon - c^\varepsilon\right) + \varepsilon \left(\varrho_0^\varepsilon - \varrho^\varepsilon\right) \boldsymbol{v}_0^\varepsilon \nabla c^\varepsilon$$
$$- \varepsilon \varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon \nabla_x c_0^\varepsilon + \varepsilon^* \varrho_0^\varepsilon \boldsymbol{v}_0^\varepsilon \nabla_x c_0^\varepsilon - \varepsilon^2 \Delta \left(c_0^\varepsilon - c^\varepsilon\right) - \varepsilon^2 \mathrm{div}_x \nabla c_0^\varepsilon - \varepsilon^2 \mathrm{div} \nabla_x c_0^\varepsilon - \varepsilon^2 \Delta_{xx} c_0^\varepsilon = 0$$

which yields after testing with $(c_0^\varepsilon - c^\varepsilon)$ and in case $\varepsilon = \varepsilon^*$:

$$\frac{1}{2}\frac{d}{dt}\int \varrho_0^\varepsilon \left(c_0^\varepsilon - c^\varepsilon\right)^2 + \int \left(\varrho_0^\varepsilon - \varrho^\varepsilon\right) \left[\partial_t c^\varepsilon + \varepsilon \boldsymbol{v}_0^\varepsilon \nabla c^\varepsilon\right] \left(c_0^\varepsilon - c^\varepsilon\right)$$
$$+ \int \varepsilon^2 \left|\nabla \left(c_0^\varepsilon - c^\varepsilon\right)\right|^2 + 2\int \varepsilon^2 \nabla_x c_0^\varepsilon \cdot \nabla \left(c_0^\varepsilon - c^\varepsilon\right) + \int \varepsilon^2 \nabla_x c_0^\varepsilon \cdot \nabla_x \left(c_0^\varepsilon - c^\varepsilon\right) = 0$$

which yields again much better estimates since the convective errors have disappeared. In particular, (B.4) reads:

$$\frac{1}{2}\frac{d}{dt}\int_{\boldsymbol{Q}_1^\varepsilon} \varrho_0^\varepsilon \left(c_0^\varepsilon - c^\varepsilon\right)^2 + \frac{1}{2}\int_{\boldsymbol{Q}_1^\varepsilon} \varepsilon^2 \left|\nabla \left(c_0^\varepsilon - c^\varepsilon\right)\right|^2$$
$$\leq \int_{\boldsymbol{Q}_1^\varepsilon} \varrho_0^\varepsilon \left(c_0^\varepsilon - c^\varepsilon\right)^2 + C_1 + C_2 \int_{\boldsymbol{Q}_1^\varepsilon} \left(c_0^\varepsilon - c^\varepsilon\right)^2 \tag{B.5}$$

with

$$C_1 = \int_{\boldsymbol{Q}_1^\varepsilon} \left(2\varepsilon^2 \left|\nabla_x c_0^\varepsilon\right|^2 + \left(\varepsilon^2 \Delta_{xx} c_0^\varepsilon\right)^2\right) \tag{B.6}$$

$$C_2 = 1 \tag{B.7}$$

Note that the error is of the same order as for the first approach but the sources of errors are less.

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