

MODELLING OF INTERFACES IN UNSATURATED POROUS MEDIA

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Abstract. In this contribution we discuss interface conditions for unsaturated flow in porous media. Typical applications are subsurface flow and technical applications like fuel cells. After an analysis of suitable interface conditions at the contact interface of two porous materials of different kind, we introduce a model for outflow boundary conditions at the interface of a porous material with open space. Finally, we discuss an existence result for unsaturated flow, supplemented with the outflow conditions.

1. Introduction. Our objective in this contribution is the discussion and the analysis of boundary conditions for unsaturated two phase flow in porous media on a macroscopic level. Examples for two phase flow in porous media are the simultaneous transport of water and oil, water and air, or any liquid together with any gas. Such flow processes occur for example in groundwater modelling, oil recovery, and environmental problems. In addition, they are of great importance in industrial applications, such as filter processes, flow through catalysts, or the gas and water flow within the diffusion medium of a fuel cell.

If one of the fluid phases is gas and the other is a liquid, in many physical situations the variations in the gas pressure can be neglected in comparison with the variations of the liquid pressure. In this case one speaks of an unsaturated flow process and models the evolution by neglecting the pressure driven motion of the gas phase. In this article we concentrate on such unsaturated flow; for simplicity of the presentation we assume that the liquid phase is water.

Our interest are unsaturated flows in situations where the porous medium is in contact with either another porous medium (with differing flow properties), or — and this is even more important — if it is in contact with an open space filled by one fluid phase. An example of such a problem is the gas and water flow within the porous diffusion layer of a fuel cell, which is in contact with a free flow in the supplying gas channels. The geometry of a fuel cell system is displayed in Figure 5.

Bulk equations. Before we turn our attention to interface and boundary conditions for unsaturated flow, let us introduce the bulk equations for two phase flow and unsaturated flow in a porous media (see [3, 6]). To fix notations we denote the region occupied by the porous material by $\Omega \subset \mathbb{R}^n$. The macroscopic behaviour of

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two phase flow is characterized by the pressures $p_\alpha(x, t)$, $\alpha = w, g$ of the water and the gas phase, the macroscopic phase velocities $v_\alpha(x, t)$, $\alpha = w, g$, and the saturation $s(x, t)$ of the water phase which is defined as the volume fraction of pore space occupied by water. As we assume that the pore space is fully occupied with water and gas, the gas saturation is given by $1 - s$.

The first model assumption is that the phase velocities are given by Darcy's law as

$$v_\alpha(x, t) = -k_\alpha(s) \nabla p_\alpha. \quad (1)$$

The bulk equations for two phase gas–water flow are then given by the conservation law for the two materials and read

$$\partial_t s = \nabla(k_w(s) \nabla p_w) + f_w, \quad (2)$$

$$\partial_t(1 - s) = \nabla(k_g(s) \nabla p_g) + f_g. \quad (3)$$

Here, $f_\alpha(x, s)$, $\alpha = w, g$ are sources and $k_\alpha(x, s)$, $\alpha = w, g$ denotes effective permeabilities of the water or gas phase, respectively. Note that for simplicity we assumed a constant porosity of the material such that all quantities are rescaled with respect to the porosity. In order to close the system we assume a material law for the capillary pressure $p_c := p_w - p_g$,

$$p_w - p_g = p_c(s) \quad (4)$$

for some given function p_c , which might also depend on the position in space, $x \in \Omega$. This law is motivated by the pore scale dynamics: The Laplace law of surface tension implies that the pressure difference depends linearly on the mean curvature of the interfaces between water and gas inside the microscopic pores. The curvature of these free boundaries depends on the typical size of the pores where interfaces are located. This, in turn, is a quantity that depends on the saturation, which motivates law (4). Regarding analysis of two phase flow equations we refer to [7], [5], and the references therein.

In the situation of unsaturated flow, we assume $p_g = \text{const}$, such that $\nabla p_w = \nabla p_c(s)$. This results in the so called Richards equation for unsaturated flow with unknown water saturation s ,

$$\partial_t s = \nabla \cdot (k(s) \nabla p) + f, \quad p \in p_c(s). \quad (5)$$

In Figure 1 the typical behaviour of the permeability – saturation, and of the capillary pressure – saturation relationship is displayed for two different materials. Note that with our notation the capillary pressure is positive for a hydrophobic material and negative for a hydrophilic one. A material that consists of a mixture of hydrophilic and hydrophobic parts may exhibit a hydrophilic or hydrophobic macroscopic behaviour depending on the water saturation (see [13]). A $p_c - s$ curve for such mixed materials is displayed on the right hand side of Figure 1. In all those cases the water permeability is zero below some critical residual saturation $s = a$. This reflects the physical situation where water pools are contained in the porous material that are not connected through pores any more (we neglect that the same effect may occur on the right end of the interval). Thus, no water flow is possible and we denote such regions (with $s \leq a$) as dry regions. The capillary pressure tends to minus infinity for s approaching a from above, and it is not defined any more in dry regions. On the other hand, we assume that for $s \rightarrow 1$ the capillary pressure either tends to plus infinity, or that it converges to a finite value. In the latter case we regard it as a multivalued function in $s = 1$, i.e. $p_c(1) = [p_*, \infty)$.

The multivalued character not only simplifies notations in the interface conditions, but it also reflects a physical fact, namely that any high pressure can be realised in a saturated medium. In many applications one uses the inverse relation, $s = \Theta(p)$, with $\Theta = p_c^{-1}$. In this formulation, Θ is defined on the whole real axis and yields a unique saturation for all pressure values.

Regarding a classical existence results for the unsaturated flow equations we refer to [1].

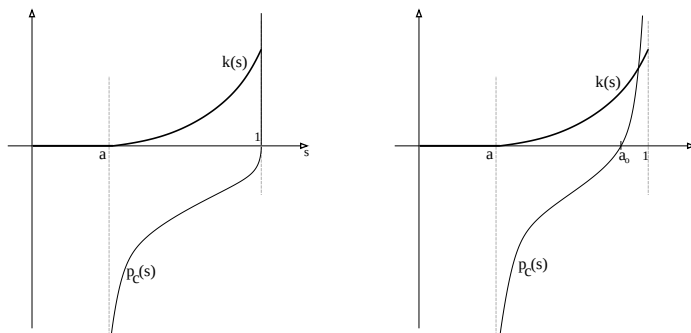


FIGURE 1. Possible shapes of the functions $p_c(s)$ and $k(s)$, a hydrophilic material on the left, a mixed material on the right. In the hydrophilic case, at a vanishing exerted pressure $p = 0$, the material is completely filled with water, $s = 1$. In this case, the capillary pressure is multivalued, $p_c(1) = [0, \infty)$. In the mixed material there are hydrophobic regions inside the material that are getting filled with water only when a positive pressure is exerted.

We note that in a saturated material (i.e. $s = 1$), the unsaturated flow equation reduces to the linear Darcy equation,

$$-\nabla \cdot (k \nabla p) = f, \quad (6)$$

with a fixed permeability $k = k(1)$.

Methods of measuring the capillary pressure – saturation relationship.

We will now describe two traditional methods for measuring the capillary pressure – saturation relationship. The first one is called *desorption method*, the second one is the *centrifuge method* (see [9]). Both methods are schematically displayed in Figure 2 and 3. We recall these experiments in order to emphasize that the interpretation of the experiment needs an understanding of interface conditions — in one case between the porous medium and a membrane, in the other between the porous medium and open space.

In the desorption method, the porous sample under investigation rests on a semi-permeable membrane which allows the water phase to flow through, but not the gas phase. The surrounding of the sample is occupied by gas which is kept at a controlled pressure. Instead, the water phase may exit the sample through the membrane and is thus in contact with the atmospheric pressure below the membrane. For each defined pressure of the gas, the system tends to an equilibrium situation where water flow stops and the amount of water remaining in the sample can be measured. Altering the pressure of the gas yields the relation between capillary pressure and saturation.

In the centrifuge method, the sample is first saturated with the water phase and then centrifuged in a container, surrounded by gas. At constant speed of rotation the amount of water that leaves the porous sample is measured. From this measurement the capillary pressure – saturation relationship can be computed.

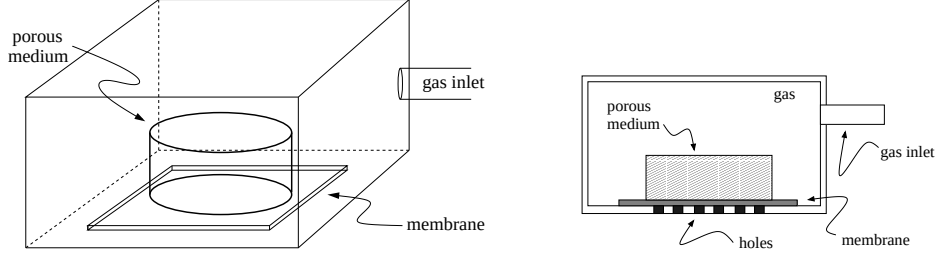


FIGURE 2. The desorption method.

Outline of this contribution. In the next section we are going to present and discuss classical interface conditions for two phase flow, when two porous media with differing material properties are in contact. In a next step, we introduce suitable boundary conditions for the outflow of water from an unsaturated porous medium into open space filled with either water or gas. Finally, in Section 3, we discuss an existence result for the Richards equation, supplemented with the outflow boundary condition from Section 2.

2. Interface conditions. We are concerned with appropriate model equations in the case that the boundary of the porous material is (i) an interface with another porous material and (ii) an interface with open space, filled with either gas or liquid. An example where the interface conditions are of utmost importance is the effect of oil trapping, see [12] and the references therein.

2.1. Contact of two porous materials. Let us first look at interfaces where two porous materials of different kind are in contact. On the interface, two transmission conditions are required. Physically, these are the continuity of the fluid pressures (balance of forces) and the continuity of the flux (conservation of mass). For a derivation of these conditions we refer to [3] and [4]. We note that in the situation of unsaturated flow also the gas phase has a constant pressure across the interface. With the notation of Section 1 this yields

$$p|_{\text{side 1}} = p|_{\text{side 2}}, \quad (7)$$

$$n \cdot (k(s)\nabla p)|_{\text{side 1}} = n \cdot (k(s)\nabla p)|_{\text{side 2}}, \quad (8)$$

where n denotes a unit outer normal to the material interface.

As the capillary pressure curve is a material property that differs from material 1 to material 2, condition (7) might enforce a jump of the water saturation s across the material interface. In the case that all expressions below are single valued, the jump is determined by the relation

$$s|_{\text{side 2}} = p_c^{-1}|_{\text{side 2}}(p_c|_{\text{side 1}}(s|_{\text{side 1}})),$$

in which the indices 1 and 2 may also be exchanged. In Figure 3 the determination of the jump condition for s is sketched for different materials on either side.

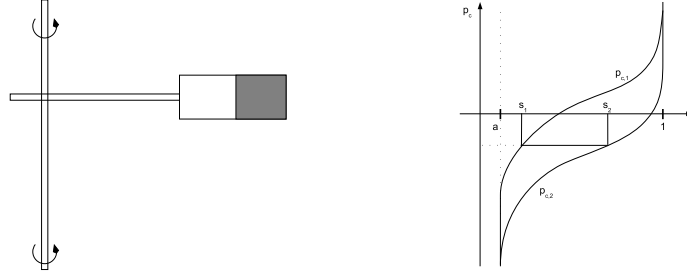


FIGURE 3. Left: Illustration of the centrifuge method to determine the capillary pressure law. Right: Diagram of the capillary pressure curves for two mixed porous media of different kind, and determination of the saturation jump at the interface.

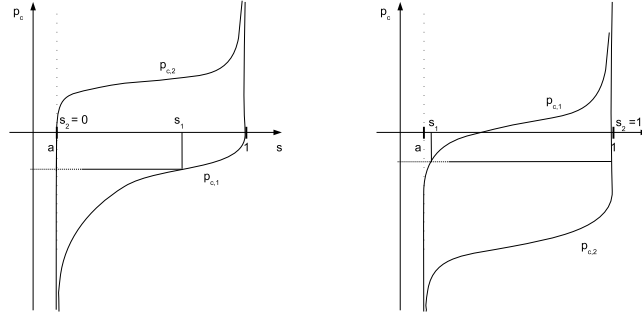


FIGURE 4. Two extreme cases for the interface condition. On the left, the contact of medium 1 with a very hydrophobic material, on the right, the contact with a very hydrophilic material.

It is interesting to discuss three special cases in which the interface condition does not reduce to a jump condition for the saturation, but to either a Neumann boundary condition, a Dirichlet boundary condition, or a different interface condition. For simplicity we assume that the value of a is the same for both materials.

A. Contact with a very hydrophobic material. Let material 2 be very hydrophobic in comparison with material 1, to be precise, let $p_{c,1}(s) \in p_{c,2}(a)$ for all values $s \in (a, 1)$. In this case, the jump relation for the saturation always yields $s = a$ in material 2. Thus no water is able to penetrate into material 2 and hence a no flux Neumann boundary condition is realized (see left of Figure 4).

B. Contact with a very hydrophilic material. On the other hand, let material 2 be very hydrophilic in comparison with material 1 such that the jump relation for the saturation always yields $s = 1$ on side 2. Thus material 2 is filled with water only and the flow in material 2 can be modelled with the Darcy equation (6) (see right of Figure 4).

C. Contact with a thin hydrophilic material. Let us assume the situation of B and, in addition, that the hydrophilic material 2 is very thin, just as in the desorption measurement method. In this case, the water pressure in material 2 can be prescribed by the surrounding pressure of material 2 and hence a Dirichlet condition

$p = p_{out}$ is realized at the interface to material 1. To make the argument complete, it must be argued as in the next subsection that the pressure in the membrane indeed coincides with the outside pressure.

2.2. Contact of a porous material with a gas surrounding. We are presenting an argument which provides the outflow boundary conditions. The conditions are used e.g. in the analysis of [2], for another description of the droplet effect we refer to [8], [10].

The droplet argument. We have to analyze the pore-scale situation; in our description we assume that the water is hydrophilic, but the arguments carry over to a hydrophobic material. In the hydrophilic case, inside the material, the small pores are filled with water, the large pores with air, both phases occupy a connected set in the pore space. Furthermore, both phases are in contact with the boundary of the medium. At the end-points of pores that are filled with gas, the equality of the gas pressures ensures the constant gas pressure inside the medium. Interesting are those points at the boundary of the medium, where a water filled pore ends. Two cases may occur.

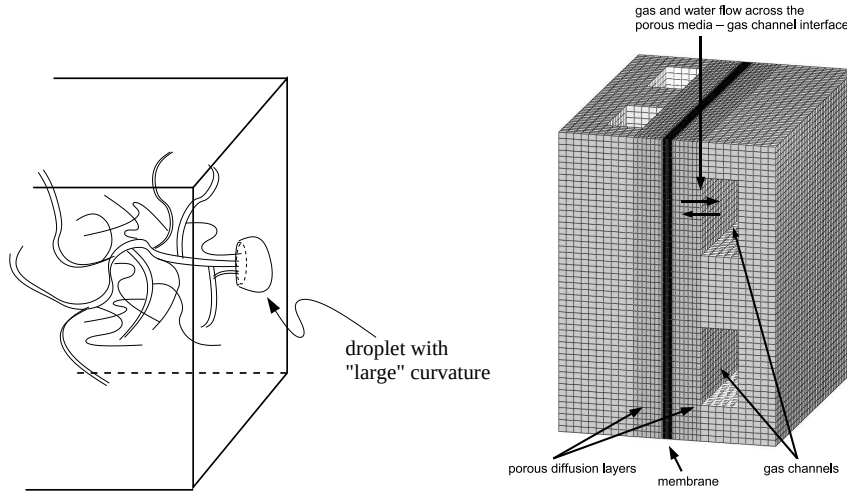


FIGURE 5. Left: Illustration of the droplet argument. The water drop sits at the macroscopic boundary of the material and has a large curvature in comparison with the water – air interfaces inside the capillaries. Right: Computational grid of a fuel cell segment.

(i) At all those points, the pore radius is so small that the water is kept inside the pore due to a high curvature of the water-gas interface. In this case, no water leaves the medium.

(ii) At some of those points, the water leaves the pore into the void space. In this case, a droplet forms as indicated in Figure 5. Since the drop is large compared to the pore scale, the curvature is small compared to the curvature of interfaces inside the pores. This means that the pressure difference between water phase and gas phase vanishes.

Effective equations. Based on the above considerations it is now easy to complete the outflow conditions. We claim that we should impose as effective equations

$$v \cdot n \geq 0, \quad (9)$$

$$p \leq 0, \quad (10)$$

$$(v \cdot n) \cdot p = 0. \quad (11)$$

Condition (9) is clear since from the gas surrounding no water can enter the porous medium. Regarding (10) we note that in the physical situation of (ii) we have a pressure difference $p_w - p_g = 0$, in our normalization $p = 0$. A higher pressure can not be achieved: A pressure $p > 0$ would result in a fast outflow of water until the pressure is fallen to $p = 0$. Finally, equation (11) reflects the fact that we have either the situation (i) and therefore $v \cdot n = 0$, or situation (ii) and therefore $p = 0$.

Remark on hydrophobic materials. The above reasoning regarding (10) fails in the case of a hydrophobic material, i.e. for $p_c^{-1}(0) = a$. In this case we expect that water leaves fastly the medium, at least those pores that are close to the boundary. But once we have a low saturation in the vicinity of the boundary, the low permeability inhibits the flow towards the boundary. The boundary conditions in this case are not clear.

2.3. Contact of a porous material with water surrounding. As a last case we have a look at boundary conditions in the case that the medium is immersed in water. Since the water filled pores are in contact with the outside water, the pressure p must coincide with the outside pressure, we find a Dirichlet condition $p = p_{out}$. As a consequence, we find the boundary condition of a prescribed saturation $s = p_c^{-1}(p_{out})$.

We emphasize that this model must be applied with care. The model is only applicable as long as the unsaturated flow assumption of a constant gas pressure remains satisfied. In particular, keeping the pressure p_{out} of the outside water below the air pressure $p_g = 0$ will result in a constant outflow of air and in a gradient in the air pressure. In this case, the two-phase flow equations must be used.

3. Existence result via regularization. In this section we refer to results obtained in [11] and sketch in a simplified form the idea for the derivation of the outflow boundary condition. We assume that $k = k(s)$ and $p_c = p_c(s)$ satisfy appropriate assumptions, which are met e.g. if k grows quadratically on $s \in [a, 1]$ and p_c does not grow too fast. We furthermore assume that $k_\delta \approx k$ and $\rho_\delta \approx p_c$ below are chosen appropriately. Here, the main condition is that the convergence $k_\delta \rightarrow k$ is fast.

Theorem 1. *Let $T > 0$, let the boundary $\partial\Omega$ be decomposed in a Neumann boundary Σ_N , a Dirichlet boundary Σ_D , and an outflow boundary Σ , and let the data p_{in} and s_0 satisfy appropriate assumptions. Let (s_δ, p_δ) be the solutions of the regularized problem (21). Then, for a subsequence $\delta \rightarrow 0$ and appropriate limiting functions, there holds with $\Omega_T = (0, T) \times \Omega$*

$$s_\delta \rightarrow s \text{ weakly-}^* \text{ in } L^\infty(\Omega_T), \quad (12)$$

$$v_\delta \rightarrow v \text{ weakly in } L^2(\Omega_T), \quad (13)$$

$$k_\delta^2(s_\delta)p_\delta \rightarrow k^2(s)p \text{ weakly in } L^2(\Omega_T), \quad (14)$$

The limits satisfy

$$\partial_t s = -\operatorname{div} v + f(\cdot, s) \text{ in } \mathcal{D}'(\Omega_T), \quad (15)$$

$$k^2(s)v = -k^3(s)\nabla p \text{ in } \mathcal{D}'(\Omega_T), \text{ and on } \{k = 0\} \text{ holds } v = 0, \quad (16)$$

$$p \in p_c(s) \text{ a.e. in } \Omega_T, \quad (17)$$

and $s(t = 0) = s_0$ in the weak sense. The limits satisfy the original boundary conditions on Σ_N and Σ_D , and on the outflow boundary $\Sigma_T = (0, T) \times \Sigma$, with s_{out} chosen to satisfy $p_c(s_{out}) = 0$, the outflow condition

$$v \cdot n \geq 0, \quad (18)$$

$$k^2(s)p \leq 0, \quad (19)$$

$$(v \cdot n) \cdot (k^2(s)s - k^2(s_{out})s_{out}) \geq 0. \quad (20)$$

The traces in (18)–(20) exist in the sense of distributions.

We remark that the Theorem does not yield quite the desired result in the second outflow condition. The result is formally equivalent to $p \leq 0$ and $v_n \cdot (s - s_{out}) = 0$. This, in turn, coincides with our outflow condition in the case of mixed materials and for hydrophilic materials with $p_c(1) = [0, \infty)$. In cases with a strict inclusion $[0, \infty) \subset p_c(1)$ we have formally only the implication $v_n \neq 0 \Rightarrow s = s_{out} = 1$, and not the equality of the pressures.

The regularized problem. We consider the regularized problem

$$\partial_t s_\delta = -\nabla \cdot v_\delta + f_\delta, \quad v_\delta = -k_\delta(s_\delta)\nabla p_\delta, \quad p_\delta = \rho_\delta(s_\delta), \quad (21)$$

with $f_\delta(x, t) = f(x, t, s_\delta(x, t))$. On the boundary Σ_{in} we impose $p_\delta = p_{in}$, on Σ_N the Neumann condition $v_\delta \cdot n = 0$. On the outflow boundary Σ_{out} we impose the mixed boundary condition

$$v_\delta \cdot n = \frac{k_\delta(s_\delta)}{\delta}(p_\delta)_+, \quad (22)$$

with $(a)_+ = \max\{a, 0\}$ denoting the positive part.

Energy estimates. Testing the equation with u yields estimates for ∇u , but only with a weight. To be precise, we can expect from the equations estimates for the integrals

$$\int_\Omega k(s)\nabla p \cdot \nabla s \sim \int_\Omega k(s)p'_c(s)|\nabla s|^2.$$

Divergence estimate. Loosely speaking, testing the equation with $k\partial_t p \sim kp'_c\partial_t s$ yields L^2 -estimates for $k \operatorname{div} v$, that is, divergence estimates for v in a weighted L^2 -space.

We now sketch the principal idea for the derivation of inequality (20).

Lemma 1. *With $K(\xi) := k(\xi)^2\xi$ we find*

$$K(s_\delta)\operatorname{div} v_\delta \rightharpoonup K(s)\operatorname{div} v \text{ in } L^2(\Omega_T). \quad (23)$$

Sketch of proof. Let us first recall why the above statement has a precise meaning. The divergence of v is defined as a distribution, and, moreover, also $K(s)\operatorname{div} v$ is defined as a distribution, since $\nabla[K(s)]$ is an L^2 function. The claim is that this distribution is in fact representable as an L^2 -function and that the above convergence holds.

The a priori L^2 estimate is contained in the divergence estimate, since $K(\xi) \leq Ck(\xi)$ with C independent of δ . We therefore find a weakly convergent subsequence.

In order to identify the weak limit, we must exploit the evolution equation. We note that we can write the above term as

$$K(s_\delta) \operatorname{div} v_\delta = \partial_t [\bar{K}(s_\delta)],$$

where $\bar{K}$ is a primitive of K . Taking distributional limits is possible for total derivatives. To make the argument rigorous, a smoothing procedure is used to derive the equality for the limit functions. $\square$

Proposition 1. *In the sense of distributions, the boundary conditions satisfy*

$$(K(s_\delta) v_\delta \cdot n)|_{\Sigma_T} \rightharpoonup (K(s) v \cdot n)|_{\Sigma_T} + \mu \text{ in } \mathcal{D}'(\Sigma_T) \quad (24)$$

for a signed measure $\mu \in \mathcal{M}(\Sigma_T)$, $\mu \leq 0$.

Proof. We first clarify the meaning of the boundary values. We write the application to a test-function $\varphi \in C_0^\infty(\Omega_T \cup \Sigma_T)$ as

$$\int_{\Sigma_T} v_\delta \cdot n [K(s_\delta)] \varphi = \int_{\Omega_T} v_\delta \nabla [K(s_\delta)] \varphi + \int_{\Omega_T} K(s_\delta) \operatorname{div} v_\delta \varphi + \int_{\Omega_T} v_\delta K(s_\delta) \nabla \varphi.$$

The same definition can be used for $\delta = 0$, since the integrands on the right hand side are all identified with L^2 functions.

It turns out that the problems arise from the first integral, since it contains the functions v_δ and $\nabla [K(s_\delta)]$, both converging weakly. We exploit that both sequences are bounded in $L^2(\Omega_T)$, hence the product is bounded in $L^1(\Omega_T)$. We therefore find a subsequence $\delta \rightarrow 0$ and a measure ν such that

$$\nabla [K(s_\delta)] \cdot v_\delta \rightharpoonup \nu \text{ in } \mathcal{M}(\bar{\Omega}_T). \quad (25)$$

We claim that the limiting measure coincides in the interior of Ω_T with the distribution $\nabla [K(s)] \cdot v$. Indeed, for $\varphi \in C_0^\infty(\Omega_T)$ we calculate

$$\begin{aligned} 0 &= \int_{\Omega_T} v_\delta \nabla [K(s_\delta)] \varphi + \int_{\Omega_T} K(s_\delta) \operatorname{div} v_\delta \varphi + \int_{\Omega_T} v_\delta K(s_\delta) \nabla \varphi \\ &\rightarrow \int_{\Omega_T} \varphi(x, t) d\nu(x, t) + \int_{\Omega_T} K(s) \operatorname{div} v \varphi + \int_{\Omega_T} v K(s) \nabla \varphi \\ &= \int_{\Omega_T} \varphi(x, t) d\nu(x, t) - \int_{\Omega_T} \nabla [K(s)] \cdot v \varphi. \end{aligned}$$

Here, the first equality is an immediate consequence of $\varphi = 0$ on Σ , in the convergence we have used Lemma 1. We conclude that $\nu = \nabla [K(s)] \cdot v + \mu$ for some defect measure $\mu \in \mathcal{M}(\bar{\Omega}_T)$. The above calculation shows that μ is concentrated on the boundary, therefore $\mu \in \mathcal{M}(\Sigma_T)$. Regarding the sign of μ we recall that the measure ν is generated by

$$\nabla [K(s_\delta)] \cdot v_\delta = \partial_s K(s_\delta) \nabla s_\delta \cdot (-k_\delta(s_\delta) \partial_s \rho_\delta(s_\delta) \nabla s_\delta) \leq 0.$$

This sign condition implies that also the singular part μ of the measure ν is non-positive, $\mu \leq 0$. We can now derive equation (24) for the boundary values with a function $\varphi \in C_0^\infty(\bar{\Omega} \times (0, T))$.

$$\begin{aligned} &\int_{\Sigma_T} K(s_\delta) v_\delta \cdot n \varphi \\ &= \int_{\Omega_T} \nabla [K(s_\delta)] \cdot v_\delta \varphi + \int_{\Omega_T} K(s_\delta) \operatorname{div} v_\delta \varphi + \int_{\Omega_T} K(s_\delta) v_\delta \nabla \varphi \end{aligned}$$

$$\begin{aligned}
& \rightarrow \int_{\Omega_T} \varphi \, d\nu + \int_{\Omega_T} K(s) \operatorname{div} v \, \varphi + \int_{\Omega_T} K(s) v \cdot \nabla \varphi \\
& = \int_{\Omega_T} \nabla[K(s)] \cdot v \, \varphi + \int_{\Sigma_T} \varphi \, d\mu + \int_{\Omega_T} K(s) \operatorname{div} v \, \varphi + \int_{\Omega_T} K(s) v \cdot \nabla \varphi \\
& = \int_{\Sigma_T} (K(s) v \cdot n)|_{\Sigma_T} \, \varphi + \int_{\Sigma_T} \varphi \, d\mu.
\end{aligned}$$

This proves (24). $\square$

Main step in the proof of inequality (20). We can take distributional limits of the boundary values to find

$$\begin{aligned}
0 & \leq (K(s_\delta) - K(s_{out})) v_\delta \cdot n \\
& \rightarrow K(s) v \cdot n + \mu - K(s_{out}) v \cdot n \\
& \leq (K(s) - K(s_{out})) v \cdot n.
\end{aligned}$$

This was the claim in (20). $\square$

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