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Variational inequalities for modeling flow in heterogeneous porous media with entry pressure

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VARATIONAL INEQUALITIES FOR MODELING FLOW IN HETEROGENEOUS POROUS MEDIA WITH ENTRY PRESSURE
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Abstract. One of the driving forces in porous media flow is the capillary pressure. In standard models, it is given depending on the saturation. However, recent experiments have shown disagreement between measurements and numerical solutions using such simple models. Hence, we consider in this paper two extensions to standard capillary pressure relationships. Firstly, to correct the non-physical behavior, we use a recently established saturation-dependent retardation term. Secondly, in the case of heterogeneous porous media, we apply a model with a capillary threshold pressure that controls the penetration process. Mathematically, we rewrite this model as inequality constraint at the interfaces which allows discontinuities in the saturation and pressure.

For the standard model, often finite volumes schemes resulting in a nonlinear system for the saturation are applied. To handle the enhanced model at the interfaces correctly, we apply a mortar discretization method on non-matching meshes. Introducing the flux as a new variable allows us to solve the inequality constraint efficiently. This method can be applied to both the standard and the enhanced capillary model. As non-linear solver, we use an active-set strategy combined with a Newton method. Several numerical examples demonstrate the efficiency and flexibility of the new algorithm in 2D and 3D and show the influence of the retardation term.

1. Motivation. Flow processes in porous media involving two immiscible fluids need to be understood and predicted when dealing with subsurface hydro systems or industrial applications. For example, in the unsaturated zone, the spatial distribution of the water and air phase as well as their fluxes serve as a basis for modeling transport of contaminants such as pesticides or heavy metals (e.g. [7]). As examples for industrial applications in two-phase flow, the movement of fluids through a filter or the infiltration of ink into paper (see [21]) can be considered. All these applications have in common, that the porous media structure is in general highly heterogeneous. The challenges are to combine the complex multi-phase flow processes with the heterogeneity distribution of the porous media properties.

The physical-mathematical model underlying simulations of two-phase flow on the Darcy scale usually requires a constitutive relationship between (wetting phase) saturation $S_w$ and the capillary pressure $p_c$. Traditionally, one assumes that this relationship is determined under quasi-static or steady-state conditions but can be also applied to any transient flow processes fulfilling the Reynolds number criterion. However, recently some works have questioned this assumption (see e.g. [22]). The authors were able to improve numerical simulation results by applying a model which accounts for a rate dependence in the $p_c(S_w)$ function. One possibility to obtain this new capillary pressure function is adding a dynamic term to the static capillary pressure relationship (see e.g. [11, 12, 13, 14]).

One of the other current challenging questions in the modeling of two-phase flow processes is the approximation of the porous media interfaces [9, 16, 25]. The heterogeneous material leads to a possibly discontinuous saturation solution at porous media interfaces. Moreover, when considering a porous medium with entry pressure, the model needs to be enhanced. In the enhanced model, also discontinuities in the capillary pressure may occur if one side is fully water-saturated.

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In this paper, we develop a new interface model that includes capillary pressure behavior with entry pressure and heterogeneities. Here, the capillary equilibrium is replaced by an inequality constraint that holds both for penetration into and leakage from higher permeability domains. A similar model for penetration processes is given and analyzed in [23].

For the discretization, we use a mortar method combined with finite volumes on each subdomain [10, 17]. The flux through the material interfaces is introduced as a new unknown and the discontinuity condition for the saturations is imposed by a weak form of the interface condition. The resulting scheme guarantees local mass conservation.

Using a biorthogonality between fluxes (Lagrange multipliers) and pressure, the inequality constraint yields node-wise. To solve the resulting inequality system, an active set strategy is used [18, 19]. The inequality is written in terms of a non-smooth equality relationship and a semi-smooth Newton method is applied. Then, in each iteration step, a conservation equation with given boundary conditions at the interface has to be solved.

The following sections are organized as follows. In section two, the model equations are presented and the behavior at material interfaces is discussed. Based on this, the new model including entry pressure is written as a variational inequality. In the third section, we develop a mortar finite volume discretization for this model and present the active set algorithm. In the last section, we discuss the new model on selected numerical examples. We consider the influence of the retardation term as well as the effect of the inequality on the numerical solution.

2. Physical-mathematical model. In this section, we present the mathematical model describing two-phase flow in a heterogeneous porous media. For a more detailed derivation and a good overview, we refer to the textbooks [2, 3, 15].

We consider an incompressible two-phase flow process in heterogeneous porous media. For simplicity, we assume no source/sink term and no gravity influence which coincides with the case of a horizontal flow without outer influences. In our model of two-phase flow in porous media, we have a wetting phase \((\alpha = w)\) and a non-wetting phase \((\alpha = n)\). The mass balance of each phase is given by

\[ \phi \frac{dS_\alpha}{dt} + \text{div} \, v_\alpha = 0, \quad \alpha \in \{w, n\}, \quad x \in \Omega, \]  

where \(v_\alpha\) is the Darcy velocity obtained from the extended Darcy’s law, i.e.,

\[ v_\alpha = -\left( \lambda_\alpha K \nabla p_\alpha \right). \]

Here, \(S_\alpha\) describes the saturation and \(p_\alpha\) the pressure of the phase \(\alpha \in \{w, n\}\), \(\phi\) and \(K\) the porosity and permeability of the soil matrix, respectively, and the mobility \(\lambda_\alpha\) is defined by \(\lambda_\alpha := \frac{\mu_\alpha}{k_{ro}}\), where \(k_{ro}\) is the relative permeability function and \(\mu_\alpha\) the viscosity of each phase. For simplicity of notation, we assume that the computational domain \(\Omega\) is split into two subdomains \(\Omega_m\) and \(\Omega_s\) and that \(\phi\) and \(K\) are constant on each subdomain. As it is usual in the context of mortar finite elements, \(\Omega_s\) stands for the slave side and \(\Omega_m\) for the master side. The interface between \(\Omega_s\) and \(\Omega_m\) is denoted by \(\Gamma\) and the normal vector on \(\Gamma\) oriented towards \(\Omega_s\) is called \(n_\Gamma\). For the moment, the choice of the master and slave side is arbitrary but should be fixed. We note that problem settings with more than two subdomains can be easily treated within the same framework.
To close the system, we need two additional supplementary equations. The first one is the saturation balance,

$$\sum_{\alpha=w,n} S_{\alpha} = 1,$$

and the second one describes the relation between the pressures,

$$p_c = p_n - p_w,$$

where $p_c$ is a given capillary pressure-saturation function.

Traditionally it is assumed that a unique relation between $p_c$ and $S_n$ exists independently of the flow conditions as long as hysteretic effects can be neglected. Recently, this assumption has been questioned and alternative formulations have been suggested. For example, the extended $p_c$ relationship by Hassanizadeh and Gray [12]. In this paper, we incorporate these ideas of different $p_c$-relationships and consider an enhanced capillary pressure-saturation model. This model includes on one hand the possibility to have a material-specific entry pressure and on the other hand is able to reflect dynamic capillary effects by adding a dynamic retardation term [11, 12, 13, 14]. Hence, the capillary pressure is then assumed to be of the form

$$p_c = p_c^{\text{stat}} + \tau \frac{dS_n}{dt},$$

with the dynamic retardation factor $\tau \geq 0$.

On each subdomain, we assume that the static capillary pressure (i.e. the capillary pressure under the assumption $\tau = 0$) $p_c^{\text{stat}} : (0,1) \rightarrow \mathbb{R}$ fulfills the following conditions:

- $p_c^{\text{stat}}$ is continuously differentiable on $(0,1)$.
- $p_c^{\text{stat}}$ is strictly increasing with respect to $S_n$.
- $p_c^{\text{stat}} \rightarrow p_c^{\text{entry}}$ for $S_n \rightarrow 0$.

We remark that in Van-Genuchten capillary pressure models, a regularized static capillary pressure is used that ensures $p_c^{\text{entry}} = 0$ and hence a continuity condition for $S_n = 0$ at both sides. However for $S_n = 0$, only the wetting phase is present, and the capillary pressure has no physical meaning. In contrast to the Van-Genuchten model, Brooks-Corey type models have different entry pressures for each material. The capillary model under consideration is therefore able to reflect the situation without regularization. In the following, we assume that the domains are split into master and slave subdomains such that $p_c^{\text{master}} \geq p_c^{\text{slave}}$, i.e., the entry pressure of the slave domain is higher than the one of the master domain.

Having specified the problem setting and the material parameters, we are now able to write the evolution equations describing the flow process in each subdomain. To get a decoupled set of equations equivalent to the two-phase system (2.1), we use
a fractional flow formulation. We note, that in contrast to standard model equations, we use a formulation based on the non-wetting saturation $S_n$. This choice simplifies the description of the behavior at material interfaces.

For the total velocity defined by $v_t := v_w + v_n$, we get the pressure equation,

$$ \text{div} v_t = 0, $$

and for $S_n$ the saturation equation,

$$ \phi \frac{dS_n}{dt} + \text{div} v_n = \phi \frac{dS_n}{dt} + \text{div} \left( f(S_n) v_t - \bar{\lambda}(S_n) K \nabla p_c \right) = 0, \quad (2.2) $$

where the fractional flow function $f$ is defined by $f = \frac{\mu_w}{\lambda_n + \lambda_m}$ and $\bar{\lambda} = \frac{\mu_n}{\lambda_n + \lambda_m}$. These equations hold in each subdomain with the given material parameters $K, \phi$ and capillary pressure relationship.

2.1. Material interfaces. In addition to the evolution equations that hold on each subdomain, interface conditions are needed which describe the behavior at the interface $\Gamma$. In standard models, two physical continuity conditions are used: the continuity of Darcy’s flux $v_\alpha \cdot \nu_\Gamma$ which guarantees conservation of mass and the continuity of the pressures $p_\alpha$ for $\alpha \in \{w, n\}$ which guarantees balance of forces. However, the last conditions can be weakened and should be only fulfilled if the phase under subject is present at both sides of the interface. To specify the interface conditions for the more general case of composite materials with entry pressure, we take a closer look at the behavior at the interface.

The continuity of Darcy velocities in normal direction, i.e., $v_\alpha \cdot \nu_\Gamma$, can be derived from the assumption that the time derivative $\frac{dS_n}{dt}$ of the saturation is bounded. Then, integrating equation (2.1) in a small neighborhood of the interface leads to a continuous $v_\alpha \cdot \nu_\Gamma$. As a consequence, $v_t \cdot \nu_\Gamma$ is also continuous. This holds for all capillary pressure relationships and therefore also for the enhanced model we consider.

For a mathematical derivation of the capillary pressure relationship, we use the results obtained by De Neef [9]. Here, a regularization technique is used to get conditions for heterogeneous materials including entry pressure. We recall that $\Omega_a$ is the side with the higher entry pressure, i.e., $p_{c,\text{entry}}^w \geq p_{c,\text{entry}}^m$. For the capillary pressure the following conditions are obtained:

$$ p_c^s = \begin{cases} p_m^w & p_m^w \geq p_{c,\text{entry}}^w, \\ p_{c,\text{entry}}^w & p_m^w < p_{c,\text{entry}}^w. \end{cases} $$

This condition is now rewritten in terms of an inequality constraint. First, we see that $p_c^w \geq p_m^w$ always holds. Moreover, a straightforward calculation gives $p_c^w - p_m^w \leq p_{c,\text{entry}}^w - p_{c,\text{entry}}^m$. Putting these two conditions together, we obtain

$$ [p_c^\text{entry}] \geq [p_c] \geq 0, $$

where $[p_c] := p_c^w - p_m^w$ denotes the jump of the capillary pressure. Moreover, we find that $[p_c] \neq 0$ directly implies $p_c^w = p_{c,\text{entry}}^w$ which is equivalent to $S_n^w = 0$. Hence, we obtain the complementary condition

$$ [p_c] S_n^w = 0. $$

To get a unique solution, we have to add an inequality constraint for the saturation as well. Here we take the physical condition of non-negative saturations,

$$ S_n^w \geq 0. $$
Putting all constraints together, we obtain for heterogeneous materials with entry pressures at the interface \( \Gamma \):

\[ [p_c^{\text{entry}}] \geq [p_c] \geq 0, \quad S_n^* \geq 0, \quad [p_c]S_n^* = 0. \]

The first condition bounds the jump of the capillary pressure for \( S_n^* = 0 \). The constraint \([p_c] \geq 0\) allows the capillary pressure at the master side to be lower than or equal to the one of the slave side, i.e., a situation where the entry pressure of the slave side is not yet reached. The condition \([p_c]^{\text{entry}} \geq [p_c]\) controls the situation for \( S_n^* = 0 \) and ensures that in this case \( p_c^e < p_c^{\text{entry}} \). We note that the complementary condition \([p_c]S_n^* = 0\) implies \( S_n^* = 0 \) for \( p_c^e \neq p_c^{\text{entry}} \).

**Remark:** Similar interface conditions can be obtained for a coupled formulation, which can be used instead of the fractional flow formulation. For example, using \( S_n \) and \( p_w \) as unknowns, additionally to the capillary inequality constraints (2.3), we get a continuity condition for the wetting pressure, \([p_w] = 0\).

### 2.2. Variational inequality.

We now write equation (2.2) in a weak form and incorporate the interface constraints (2.3). The main idea is to use the continuous flux \( \nu_n \cdot \nu_T \) at the interface \( \Gamma \) as new unknown and write the interface conditions in a weak form with suitable test spaces. This leads to a variational inequality that describes the behavior of heterogeneous porous media in the presence of entry pressures.

First, we introduce some regularity assumptions. We define the space \( V \) by \( V := H^1(\Omega_n) \times H^1(\Omega_s) \), the space \( W \) as \( W := H^{1/2}(\Gamma) \) and \( M := W' \) the dual space of \( W \) and assume that \( S_n \in V \), \( v_n|_\Gamma \cdot \nu_T \in M \). To simplify notation, we use in the following \( S \) instead of \( S_n \) and \( v \) instead of \( v_n \). Then, the integral form of (2.2) reads

\[ \int_V \phi \frac{dS}{dt} + \int_{\partial V} v \cdot \nu_V = 0, \]

for all control volumes \( V \subseteq \Omega_k \), \( k = s, m \), where \( \nu_V \) is the outer normal of \( V \). Here, \( v \) is given by

\[ v = f(S)v_t - \lambda(S)K\nabla p_c, \]

and therefore depends on \( S \) and \( p_c \) (which itself depends on \( S \) and \( \frac{dS}{dt} \)). Let us define \( \Lambda \) by \( \Lambda := v|_\Gamma \cdot \nu_T \). We remark that on \( \Gamma \), \( v \cdot \nu_V = \Lambda(\nu_V \cdot \nu_T) \) holds, see Figure 2.2. The term \( \nu_V \cdot \nu_T \) is \( +1 \) if the control volume \( V \) is on the master side and \( -1 \) if it is on the slave side. The integral equation then reads:

\[ \int_V \phi \frac{dS}{dt} + \int_{\partial V \setminus \Gamma} v \cdot \nu_V + \int_{\partial V \cap \Gamma} \Lambda(\nu_V \cdot \nu_T) = 0 \quad V \subseteq \Omega_k. \]

We see that here \( \Lambda \) enters like a flow boundary condition.

To write the interface conditions (2.3) in a weak form, we have to define suitable testspaces. We start with the conditions \([p_c] \geq 0\) and \([p_c]S_n^* = 0\). The last condition implies that we have to consider the inequality constraint only for \( S_n^* = 0 \). We therefore define the subset \( \Gamma_S \) of \( \Gamma \) and its complement \( \Gamma_S^c = \Gamma \setminus \Gamma_S \) by the conditions \( S_n|_{\Gamma_S} = 0 \) and \( S_n|_{\Gamma_S^c} > 0 \), see Figure 2.2. Then the test space \( M(S) \) is defined by

\[ M(S) := \left\{ \zeta \in M : \int_{\Gamma_S} \zeta \cdot \xi \geq 0, \quad \xi \in W, \xi \geq 0 \right\} \]
We note that the space $M(S)$ yields the constraint $\zeta > 0$ in a weak form on $\Gamma_S$. Therefore the weak form of the conditions $[p_c] \geq 0$ and $[p_c]S^s = 0$ in (2.3) can be written by testing with an element in $M(S)$ as

$$\int_{\Gamma_S} [p_c] : \zeta \geq 0 \quad \zeta \in M(S).$$

The choice of the space $M(S)$ automatically ensures that the complementary condition $[p_c]S^s = 0$ holds in a weak form. As no positivity constraint for $M(S)$ is used on $\Gamma_S$, we can test with $\zeta$ such that $\zeta|_{\Gamma_S} = -\zeta|_{\Gamma_S}$ and obtain

$$\int_{\Gamma_S} [p_c] : \zeta \geq 0, \quad -\int_{\Gamma_S} [p_c] : \zeta \geq 0,$$

which implies

$$\int_{\Gamma_S} [p_c] : \zeta = 0 \quad \zeta \in M.$$

For the condition $[p_c^{\text{entry}}] \geq [p_c]$, we define

$$M^+ := M(0) = \left\{ \zeta \in M : \int_{\Gamma_S} \zeta : \xi \geq 0, \quad \xi \in W, \xi \geq 0 \right\},$$

which yields the aforementioned positivity constraint independent of $S$ and get the weak formulation

$$\int_{\Gamma_S} ([p_c^{\text{entry}}] - [p_c]) : \zeta \geq 0 \quad \zeta \in M^+.$$

Putting all together, we finally obtain the following variational inequality: Find $S, \Lambda$ such that

$$\int_V \frac{dS}{dt} + \int_{\partial V \setminus \Gamma} \nu \cdot \nu V + \int_{\partial V \cap \Gamma} \Lambda (\nu \cdot \nu V) = 0 \quad V \subseteq \Omega_k, \quad (2.4)$$

$$\int_{\Gamma} ([p_c^{\text{entry}}] - [p_c]) : \zeta \geq 0 \quad \zeta \in M^+, \quad (2.5)$$

$$\int_{\Gamma} [p_c] : \zeta \geq 0 \quad \zeta \in M(S). \quad (2.6)$$
We remark that several nonlinearities remain in this equation. Besides the inequality constraints, the constitutive relationships \( p_c^{\text{stat}} \) and \( \lambda_w, \lambda_n \) in general depend nonlinear on \( S \). The capillary pressure relationship not only enters in the evolution equation but also in the inequality constraints.

3. Discretization and active set strategy. In this section, we apply a suitable discretization scheme in time and space on the saddle point problem (2.4)-(2.6).

Here we proceed in a similar order as in the derivation of the model. After applying a suitable time integration scheme, we first discretize the evolution equation using finite volume techniques. To discretize the interface conditions, discrete ansatz and testspaces equivalent to the continuous counterparts are defined. To solve the remaining discrete inequality constraints, we propose an active set algorithm. Then, in each iteration step, a (nonlinear) equation system has to be solved.

3.1. Time discretization. For the time discretization, we use a standard implicit Euler scheme. Denoting the time index by \( n \), the time-discretized formulation reads: For given \( S^n \), find \( S^{n+1}, \Lambda^{n+1} \) such that

\[
\int_V \frac{S^{n-1} - S^n}{\Delta t} + \int_{\partial V \setminus \Gamma} v(S^{n+1}, S^n) \cdot \nu - \int_{\partial V \cap \Gamma} \Lambda^{n+1} (\nu \cdot \nu_T) = 0 \quad V \subseteq \Omega_k, \quad \mu \geq 0 \quad \mu \in \mathcal{M}^+, \quad \mu \in \mathcal{M}(S^{n+1}).
\]

Here, the time-discretized Darcy-velocity \( v \) is defined by

\[
v(S^{n+1}, S^n) := f(S^{n+1}) v_t + \bar{\lambda}(S^{n+1}) K \nabla p_c(S^{n+1}, S^n),
\]

and the capillary pressure function is discretized by

\[
p_c(S^{n+1}, S^n) := p_c^{\text{stat}}(S^{n+1}) + \frac{S^{n+1} - S^n}{\Delta t}.
\]

We note that the test-space \( \mathcal{M}(S^{n+1}) \) is also used with respect to the timestep \( n+1 \), hence the following complementary condition is fulfilled:

\[
\int_{\Gamma_{S^{n+1}}} [p_c(S^{n+1}, S^n)] \cdot \zeta = 0 \quad \forall \zeta \in \mathcal{M}.
\]

3.2. Space discretization. For the space discretization, we use a vertex based finite volume discretization to ensure the local mass-conservation of our approach and define an appropriate numerical flux function on each subdomain, see, e.g., [6, 15, 20] for details about finite volume discretizations. The basic idea of this discretization is to use a dual mesh for the finite volume scheme and define a numerical flux that is induced by the gradients of standard finite element functions.

To define the discrete spaces and the numerical scheme, we assume that the domains \( \Omega_s \) and \( \Omega_m \) are unions of triangles and quadrilaterals in 2D or tetrahedrons and hexahedrons in 3D given by a triangulation \( T_h = T_h^s \cup T_h^m \). We note that the triangulations of \( \Omega_s \) and \( \Omega_m \) may be independent from each other. Then the dual mesh \( T_h^* \) of \( T_h \) is defined by polygons or polyhedrons, respectively, surrounding the vertices of \( T_h \). The polygons are given by the centers of gravity of the adjacent
elements and the midpoints of adjacent edges and the polyhedrons by the centers of gravity of adjacent elements and sides and midpoints of adjacent edges, see Figure 3.1. The dual mesh is considered for the slave and master side independently, and we set $T_h^* := (T_h^*)^s \cup (T_h^*)^m$.

![Primal mesh $T_h$ and dual mesh $T_h^*$ on $\Omega_h$.](image)

The discrete spaces $V_h^s$ and $V_h^m$ are defined as the Lagrange finite element spaces of first order with respect to the triangulation $T_h^*$ and $T_h^m$, respectively. The basis function associated with the node $j$ is denoted by $\varphi_j$. Integrating over elements $T$ of the dual mesh $T_h^*$ gives the following equation for the discretized saturation $S_h^{n+1} = \sum S_j^{n+1} \varphi_j$:

$$
\Phi \int_T \frac{S_h^{n+1} - S_h^n}{\Delta t} + \int_{\partial T \setminus \Gamma} F_{\text{num}} \cdot \nu_T + \int_{\partial T \cap \Gamma} A_h(\nu_T \cdot \nu_T) = 0 \quad T \in T_h^*.
$$

Here, $\nu_T$ is defined as the outer normal vector of the test volume $T \in T_h^*$.

For the numerical flux function $F_{\text{num}}$, we use a finite element approximation of $v(S_h^{n+1}, S_h^n)$ on the boundary of the dual element $T$.

$$
F_{\text{num}} := \alpha \nu_T + \beta K \nabla S_h^{n+1} + \gamma K \nabla \frac{S_h^{n+1} - S_h^n}{\Delta t}.
$$

Here, the coefficients $\alpha, \beta, \gamma$ are defined in terms of the saturation $S_h$ by:

$$
\alpha := f(S_h^{n+1}), \quad \beta := -\lambda(S_h^{n+1})(\rho_e^{\text{stat}})'(S_h^{n+1}), \quad \gamma := -\lambda(S_h^{n+1}) \tau.
$$

We note that the gradients of the finite element functions are well-defined on the boundary of the dual elements $T \in T_h^*$ because the basis functions $\varphi_j$ are polynomial on each element of the primal mesh $T_h$. As standard in finite volume schemes for convection-diffusion problems, we use an upwinding strategy on the first order term $\alpha$ depending on the flux-direction. To be more precise, the function $f$ is evaluated with respect to the nodal saturation values where the node is chosen with respect to the flow direction of $v_T$.

Having described the discrete equations in each domain $\Omega_k$, we now give the discretized form of the interface conditions. Here, we apply mortar techniques [4,
5, 26] to define suitable discrete spaces for A and test spaces for the weak inequality constraints. We remark that these methods are widely used in engineering applications and have successfully been applied to the pressure equation in porous media, see [24, 27] and the references therein.

First, we define a triangulation $\mathcal{T}_{h, \Gamma}$ of the interface $\Gamma$. Here, we use the triangulation induced by the triangulation of the slave side $\Omega_s$. The dual mesh $\mathcal{T}_{h, \Gamma}^*$ is defined the same way by using the dual mesh $(\mathcal{T}_{h}^*)^*$ of the slave side.

For the Lagrange multiplier, we use the space $\mathbf{M}_h$ of piecewise constant functions on $\mathcal{T}_{h}^*$. We note that using $\Lambda_h \in \mathbf{M}_h$, the Lagrange multiplier enters in a natural way as piecewise constant flux boundary condition in (3.1). For the discretization of the test spaces $\mathbf{M}(S)$ and $\mathbf{M}^+$, we use the dual Lagrange multiplier space $\mathbf{M}_h$ with respect to the standard finite element space. Here, the basis functions $\psi_j$ of $\mathbf{M}_h$ are chosen such that $\int_{\Gamma} \varphi_i \psi_j = 0$ for $i \neq j$. Therefore a decoupling of the degrees of freedom is possible. For details of the construction and additional information, we refer to [26].

We note that for elliptic problems, this choice of Lagrange multiplier spaces leads to an optimal order approximation of the primal variable. For a proof, one can follow the lines in [10] and use the stability of the projection onto the dual Lagrange multiplier space [26]. Moreover, we remark that other choices for the Lagrange multiplier spaces are possible, e.g., piecewise constant for both $\mathbf{M}_h$ and $\mathbf{M}_h$, see [10].

We recall that $S_h$ is defined as finite element function, $S_h = \sum_j \tilde{S}_j \varphi_j$ and $\{\psi_j\}$ are the basis functions of $\mathbf{M}_h$. Using the space $\mathbf{M}_h$, the discrete equivalent of $\mathbf{M}(S)$ is now defined as

$$\mathbf{M}_h(S_h) := \{ \zeta = \sum_j \zeta_j \psi_j \in \mathbf{M}_h : \zeta_j \geq 0 \text{ for } S_j = 0 \}.$$ 

The space $\mathbf{M}_h^+$ is defined analogously without the restriction on $S_h$. Using these test spaces, the interface conditions (2.5)-(2.6) read

$$\int_{\Gamma} ( [p^\text{entry}_c] - [p_c(S_{h,n+1}^n, S_h^n)] ) \cdot \zeta \geq 0 \quad \zeta \in \mathbf{M}_h^+,$$

$$\int_{\Gamma} [p_c(S_{h,n+1}^n, S_h^n)] \cdot \zeta \geq 0 \quad \zeta \in \mathbf{M}_h(S_{h,n+1}^n).$$

Here, $p_c(S_{h,n+1}^n, S_h^n) \in \mathbf{M}_h^+$ is defined as the finite element interpolation of $p_c$, i.e.,

$$p_c(S_{h,n+1}^n, S_h^n) = \sum_j p_{c,j} \varphi_j, \quad p_{c,j} := p^{\text{stat}}_c(S_{j,n+1}^n) + \frac{S_{j,n+1}^n - S_{j,n}^n}{\Delta t}.$$

Now we arrive at the discrete formulation for our problem with entry pressure: For a given $S_h^n$, find $S_{h,n+1}^n \in \mathbf{V}_h, \Lambda_{h,n+1}^n \in \mathbf{M}_h$ such that:

$$\Phi \int_T S_{h,n+1}^n - S_{h,n}^n \frac{\Delta t}{\Delta t} + \int_{\partial T \setminus \Gamma} F_{\text{num}} \cdot u_T + \int_{\partial T \setminus \Gamma} \Lambda_{h,n+1}^n (v_T \cdot u_T) = 0 \quad T \in \mathcal{T}_h^*, \quad (3.2)$$

$$\int_{\Gamma} ([p^\text{entry}_c] - [p_c(S_{h,n+1}^n, S_h^n)]) \zeta_h ds \geq 0 \quad \zeta_h \in \mathbf{M}_h^+, \quad (3.3)$$

$$\int_{\Gamma} [p_c(S_{h,n+1}^n, S_h^n)] \zeta_h ds \geq 0 \quad \zeta_h \in \mathbf{M}_h(S_{h,n+1}^n). \quad (3.4)$$
In this system two kinds of nonlinearities remain to solve. The first is given in terms of the variational inequality, and the second one is due to the nonlinear functions \( p_c, f \) and \( \lambda \) which appear in the numerical flux function \( F_{\text{num}} \) and the inequality constraints.

3.3. Numerical algorithm. In the rest of this section, we briefly sketch the algorithm that is used to solve the system (3.2)–(3.4). To solve the nonlinearities associated with the inequality constraints, we use an active set strategy. This method is an interpretation of a semi-smooth Newton method [19] applied to an equivalent, non-smooth equality constraint and has been successfully applied to engineering problems such as, e.g., in contact mechanics, see [1, 8, 18]. Here, we adapt these ideas to our case of heterogeneous porous media.

First, we see, that by definition of the testspaces, the interface conditions can be written as pointwise conditions for each node of the triangulation \( T_h, T \):

\[
[p_c^{\text{entry}}] - [p_c(S_h^{n+1}, S_h^n)]_j \geq 0, \quad (3.5)
\]

\[
[p_c(S_h^{n+1}, S_h^n)]_j \geq 0 \quad \text{for} \quad S_j^{n+1} = 0, \quad (3.6)
\]

\[
[p_c(S_h^{n+1}, S_h^n)]_j = 0 \quad \text{for} \quad S_j^{n+1} > 0. \quad (3.7)
\]

Here, \([\cdot]_j\) is defined by \( \int_T [\cdot]_j d_T \). We remark that the definition of \( p_c(S_h^{n+1}, S_h^n) \) and the dual Lagrange multiplier space \( M_h \) imply that these conditions on the slave side only depend on \( S_j \); moreover in the case of matching meshes on the slave and master side, we get nodewise conditions for each corresponding pair of nodes at the interface.

The idea of the active set strategy is to split the set of nodes on \( T_{h, T} \) into two sets \( A \) and \( N \) which are called active and inactive set. The sets are chosen such that for \( j \in A \), the condition \([p_c(S_h^{n+1}, S_h^n)]_j = 0\) is fulfilled, while for \( j \in N \), the condition \( S_j^{n+1} = 0 \) holds. If \( A \) and \( N \) are known, then the inequality constraints turn into equality constraints which are either the continuity of the capillary pressure or a Dirichlet boundary conditions for the saturation at the slave side. The resulting nonlinear problem then reads: Find \( S_h^{n+1}, A_h^{n+1} \) such that

\[
\Phi \int_T S_h^{n+1} - S_h^n \delta t + \int_{\partial T \setminus \Gamma} F_{\text{num}} \cdot n_T + \int_{\partial T \cap \Gamma} A_h^{n+1}(n_T \cdot n_T) = 0 \quad T \in T_h^*, \quad (3.8)
\]

\[
[p_c(S_h^{n+1}, S_h^n)]_j = 0 \quad j \in A, \quad (3.9)
\]

\[
S_j^{n+1} = 0 \quad j \in N. \quad (3.10)
\]

This equation can be solved for given sets \( A, N \) by a standard Newton approach, see, e.g., [15]. We remark that in the resulting tangential matrix, a static condensation can be applied which eliminates the Lagrange multiplier as unknown [18].

To determine the correct active and inactive set, an iterative scheme is used. In each iteration step the nonlinear equations (3.8)–(3.10) are solved by Newton’s method. Then the conditions (3.5), (3.6) and \( S_j^{n+1} \geq 0 \) are checked pointwise. If they are not satisfied, the corresponding node is changed from active to inactive and vice versa. Then the algorithm to determine \( A_{k+1} \) and \( N_{k+1} \) reads:

- Solve (3.8)–(3.10) iteratively with \( A = A_k, N = N_k \).
- Set \( A_{k+1} := \{ j \in A_k : S_j \geq 0 \} \cup \{ j \in N_k : [p_c^{\text{entry}}]_j < [p_c]_j \} \) or \([p_c]_j < 0\).
- Set \( N_{k+1} := \{ j \in A_k : S_j < 0 \} \cup \{ j \in N_k : [p_c^{\text{entry}}]_j \geq [p_c]_j \} \).

We note that the condition \( S_j \geq 0 \) has to be checked because the condition \([p_c] = 0\) can cause negative saturations on the slave side if the capillary pressure of the master side is below the entry pressure of the slave side.
To solve the fully discretized problem, we get an algorithm consisting of three nested loops: the outer loop is the time loop given by the implicit Euler discretization. For each time step an active set-loop is used to find the correct sets \( A \) and \( N \). Moreover, in each active set step the resulting nonlinear equation is solved by a Newton iteration.

Remark: A good choice to start the active set iteration is by using the active and inactive set of the last timestep. In fact, by this choice the number of active set iterations is about 2 or 3 in our applications, and therefore the computational effort is similar to problems without variational inequality condition. Additionally, loop-unrolling can be used, i.e., the Newton and active-set update is done within each iteration step.

4. Numerical simulation. In this section, we apply our scheme to different problem settings and verify the flexibility and efficiency of our algorithm. We start with model problem settings consisting of two subdomains with different material parameters and study the influence of the material parameters and flow direction at the interface. At the end of the section, more realistic settings, i.e., porous media with layers of higher permeability, are considered in 2D and 3D.

4.1. Example 1. In the first example, we consider a rectangular domain \( \Omega := (0,2) \times (0,1) \) that is divided into two subdomains \( \Omega_m := (0,1) \times (0,1) \) and \( \Omega_s := (1,2) \times (0,1) \). We consider a flow from the left to the right side and material parameters such that the entry pressure of the right side is greater than the entry pressure of the left side. The material parameters are given by \( \Phi_s = \Phi_m = 1 \) and \( K_s = 0.25 Id, \quad K_m = Id \). We assume a static capillary pressure function of Brooks–Corey type, i.e., \( p_c^{stat} = 4/(1 - S) \) and \( p_m^{stat} = 2/(1 - S) \) and \( \tau_s = \tau_m = 0 \). As relative permeability, we choose a quadratic dependency, i.e., \( k_{rn} = S^2, \quad k_{rw} = (1 - S)^2 \). The initial saturation \( S^{init} \) is given by the polynomial spline function

\[
S^{init} = \begin{cases} 
8(128x_1^4 - 48x_1^2 + 1)x_2^2(1 - x_2)^2 & x_1 \leq 0.25, \\
0 & x_1 > 0.25,
\end{cases}
\]

and as boundary conditions we use the Dirichlet boundary condition \( S = S^{init} \) on \( 0 \times [0,1] \), outflow boundary conditions on \( 2 \times (0,1) \) and homogeneous Neumann boundary conditions elsewhere, see Figure 4.1. The used grid is depicted in the right picture of Figure 4.1.

![Fig. 4.1. Example 1: left: problem setting \( \Omega \), right: grid](image)

The solution at various time-steps is given in Figure 4.2. Here we see that the solution is travelling from the left to the right. At the interface the flow is first blocked resulting in a higher saturation at the left side of the interface. As soon as the entry pressure of the right side is reached, we have penetration into the right subdomain which leads to an ongoing flow from left to right. In Figure 4.3, we take
a closer look on the infiltration process. In the left picture, the saturation at both sides of the interfaces at time $t = 0.06$ is plotted. Here, the discontinuity of the saturations, induced by the different capillary pressure relationships, can be seen. Moreover, the parts of the interface where the entry pressure of the right side has not yet been reached can easily be identified. These parts correspond to the set $\Gamma_s$. In the right picture, a cut through the domains is given. Here, two different kinds of traveling waves in the left and right subdomains can be observed. The one of the right subdomain is smoother which can be explained by the lower permeability and higher capillary pressure. At the interface the jump in the saturations given by the continuity of capillary pressure arises as the wave passes the interface.

4.2. Example 2. In the second example, we use the same setting as in Example 1 with the difference that the left and right boundary conditions and the direction of the total velocity are switched; the initial condition is mirrored with respect to $x = 1$. This means that now a flow from the medium with higher entry pressure to the medium with lower entry pressure is considered.

In Figure 4.4 the solution at different time-steps is given. A wave travelling from the right to the left can be observed. At the interface, the wave propagation proceeds almost undisturbed. As soon as the interface is reached, penetration into the left subdomain starts and the wave continues to travel. To get a better understanding,
we consider the saturation at the interface, see Figure 4.5. The saturation at the right side of the interface is zero for all time-steps. This means that at the interface a sucking effect happens: As soon as the non-wetting phase reaches the interface, it is transported to the right side. In the right picture of Figure 4.5, a cut through the domains is given. We see that the saturation at the right side converges over the time to a limit profile with saturation zero at the interface.

4.3. Example 3. In the third example, we demonstrate the flexibility of our scheme with respect to flow directions. To do so, we use the same setting as in Example 1 but here the total velocity and boundary conditions are switched at time \( t = 0.1 \). The boundary conditions are mirrored with respect to \( x = 1 \) with the difference that instead of \( S^{\text{init}} \) we impose zero Dirichlet boundary conditions at the right side. This means that we consider an example where first inflow and then outflow of the non-wetting phase is considered.

In Figure 4.6, the solution at different time-steps is depicted. Obviously, in the beginning the behavior is identical to the one of the first example. Starting from \( t = 0.1 \), the total velocity is switched and hence the flow-direction turns. Therefore, the already infiltrated non-wetting phase is again displaced by the wetting phase. Here, a similar sucking process as in Example 2 takes place which implies that the outflow process is much faster than the penetration process in this example.
We see that our model works for both flow-directions at the interface without the need to incorporate the situation into the model. In contrast to other models, both cases are reflected by the variational inequality conditions which makes our scheme quite flexible.

4.4. Example with dynamic capillary pressure. In the next example, we use the same setting as in Example 1, but include a non-zero dynamic capillary pressure relationship. Here, we use $\tau_m = 0.1$ and $\tau^s = 0.2$.

The solution at several time-steps is given in Figure 4.7. We see that the retardation term leads to a slow-down of the wave propagation process. At the same time, a saturation pooling can be observed which leads to a non-monotonous wave profile. The penetration into the right subdomain starts almost immediately as the wave reaches the interface. This effect can be explained by the enlarged capillary pressure for increasing non-wetting saturation. At the right side, again non-monotonous wave-profiles appear. The shape of these waves is strongly influenced by the penetration
process. As the penetration starts at the center of the interface, we see that the wave not only propagates in \( x_1 \) but also in \( x_2 \)-direction and therefore a non-monotonic behavior normal to the main flow direction can also be observed.

4.5. Influence of retardation parameter \( \tau \). To illustrate the influence of \( \tau \) on the flow process, we now compare the solutions to Example 3 using different values for \( \tau \). We use \( \tau^m \in \{ 0, 0.01, 0.1 \} \) and use in the right subdomain \( \tau^s = 2 \tau^m \).

![Figure 4.8](image)

**Fig. 4.8. Influence of parameter \( \tau \). First line: \( \tau^m = 0 \), second line: \( \tau^m = 0.01 \), third line: \( \tau^m = 0.1 \). Left column: cut, middle column: solution at \( t = 0.06 \), right column: solution at \( t = 0.12 \).**

The results are given in Figure 4.8. In the first line, the solution without retardation factor is given. In the second line, a small value of \( \tau \) is used, \( \tau^m = 0.01 \). Here, a small pooling effect and hence non-monotonic wave profiles can be observed; however, the propagation speed only slightly differs from the one with zero \( \tau \). For the value \( \tau^m = 0.1 \), a large effect can be observed that leads to a slower propagation at the left side.

4.6. Domain with layers. In this example, we use a more complex problem setting. Here, the domain is given by \( (0, 10) \times (0, 10) \). In the interior, we have three layers, \( \Omega_1 := (2.3) \times (1.5), \Omega_2 := (4.5) \times (5.9) \) and \( \Omega_3 := (6.9) \times (4.7) \), see Figure 4.9. \( \Omega_i, i = 1, \ldots, 3 \) act as slave domains and \( \Omega \setminus \Omega_1 \cup \Omega_2 \cup \Omega_3 \) as master domain. The material parameters are given by \( \Phi = 1 \) and \( K_1 = K_2 = 0.2 Id, K_3 = 0.5 Id \) and \( K_m = Id \). Here we use a very simple capillary pressure model, i.e., a linear relationship with different entrypressures, \( p_c^{1, \text{stat}} = p_c^{2, \text{stat}} = 10S + 2, p_c^{3, \text{stat}} = 10S + 1 \) and \( p_c^{m, \text{stat}} = 10S \). As dynamic factors \( \tau \) we consider in a first setting no dynamic term, \( \tau = 0 \) and in a second setting \( \tau = 0.1 \). As relative permeability, we choose a quadratic dependency, i.e., \( k_{rn} = s^2, k_{ru} = (1 - s)^2 \). As initial condition, we assume that both subdomains are fully water-saturated, i.e., \( S = 0 \). The boundary conditions are given by a Dirichlet boundary condition \( S = 0.5 \) on \( 0 \times [2.5, 7.5] \), outflow boundary conditions on \( 10 \times (0, 10) \) and homogeneous Neumann boundary conditions elsewhere.
The solution for $\tau = 0$ at different time-steps is given in Figure 4.10. Here, the influence of the entry pressure can clearly be seen. There is no penetration into the lower left subdomain $\Omega_1$ until the entry pressure is reached and this affects the general flow behavior. The same holds for the subdomains $\Omega_2$ and $\Omega_3$. Moreover, the pooling at the left interfaces on each subdomain remains to ensure the continuity of the capillary pressure while on the right interfaces of each subdomain $\Omega_i$ a sucking
effect is observed.

![Diagram](image_url)

**Fig. 4.11.** Solution at time $t = 0.02, 0.04, 0.06$ for $\tau = 0$ (upper row) and $\tau = 0.1$ (lower row)

Comparing the situation $\tau = 0$ with $\tau = 0.1$, see Figure 4.11, similar dynamic effects as observed in the previous examples can be seen. Here, the non-monotonous wave profile dominates in the beginning. However, the flow is much more depending on the geometry of the heterogeneities than on the dynamic retardation term in this example. This can be seen by the fact that for later time-steps there are only small differences between the two flow processes.

5. **3D example.** Finally, we consider a 3D example. The domain $\Omega$ is a cube $[0, 5] \times [0, 5] \times [0, 5]$ with two layers of higher permeability. These layers are given by $\Omega_2 = [1, 2] \times [1, 2] \times [3, 4]$ and $\Omega_3 = [1, 4] \times [1, 4] \times [1, 2]$ and act as slave domains whereas $\Omega_1 = \Omega \setminus \Omega_2 \cup \Omega_3$ is the master domain, see Figure 5.1. As material parameters we use $\Phi = 1$ and $K_1 = 1d$, $K_2 = 36d$ and $K_3 = 41d$ and the constitutive relationships are given by $p_c^{1, \text{stat}} = \frac{50}{S}$, $p_c^{2, \text{stat}} = \frac{300}{S}$, $p_c^{3, \text{stat}} = \frac{100}{S}$ and a quadratic relative permeability function, $k_{rn} = s^2$, $k_{rw} = (1-s)^2$. Here we use a dynamic capillary relationship with $\tau_1 = 2.5$, $\tau_2 = 15$, $\tau_3 = 5$. As initial condition, we assume that $\Omega$ is fully water saturated, i.e., $S = 0$ and the boundary conditions are given by outflow boundary conditions on $x_3 = 0$ and Dirichlet boundary conditions $S = 0.5$ on $[1.5, 2.5] \times [1.5, 2.5] \times \{5\}$.

The solution at different time-steps is depicted in Figure 5.2. At the top of the subdomain $\Omega_2$ a pooling is observed; however, there is no penetration into $\Omega_2$ as the entry pressure is not reached. The non-wetting phase flows around $\Omega_2$ and the front reaches the other layer, $\Omega_3$. Here the entry pressure is reached quite soon and penetration into the layer can be observed.
Fig. 5.1. 3D example: Problem setting

Fig. 5.2. Solution at time $t = 0.02 \ldots 0.12$

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