Analysis of DNAPL infiltration in a medium with a low-permeable lens

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In this paper we study the infiltration of DNAPL in a porous medium containing a single low-permeable lens. Our aim is to determine whether or not DNAPL infiltrates into the lens. A key role is played by the capillary pressure: DNAPL cannot infiltrate into the lens unless the capillary pressure exceeds the entry pressure of the lens. In the model this is reflected by an interface condition, the extended capillary pressure condition. To derive analytical approximations we first consider a steady-state DNAPL plume in a homogeneous medium. This results in an estimate of the DNAPL plume width as a function of depth, and an asymptotic solution for small saturations. Assuming that the extent of the lens is much larger than the width of the unperturbed DNAPL plume in the homogeneous medium, we derive an explicit criterion for DNAPL infiltration into the lens in terms of a critical inflow rate. A numerical algorithm is presented in which the extended capillary pressure condition is incorporated. The numerical and analytical results show good qualitative agreement.

Keywords: two-phase flow, DNAPL, low-permeable lens, capillary pressure, entry pressure, critical flow rate

AMS subject classification: 35R05, 65M06, 76T05

1. Introduction

The infiltration of Dense Non-Aqueous Phase Liquid (DNAPL) into aquifers forms a serious environmental problem. DNAPLs are organic compounds with a higher density than water; examples are chlorinated solvents used in industry. Since DNAPLs are heavier than water they easily invade the saturated zone of the subsurface, posing a threat to the ground water quality. Even small concentrations of compounds derived from typical DNAPLs can be toxicologically significant.

Several remediation techniques exist to remove DNAPL from the subsurface. The effectivity of hydraulic remediation techniques (pumping of contaminated ground water) is limited if the DNAPL has entered less-permeable regions like lenses of very fine sand. The reason is that the low-permeability zones are hardly reached, because the preferred flow path of water is in the high-permeability zones. This applies equally well to other remediation techniques like in situ biodegradation and surfactant enhanced dissolution, since both techniques use water for transport of the remediating substances. Excavation is often not feasible because of the great infiltration depth. So lenses of low permeability infiltrated by DNAPL may form persistent sources of ground water contamination. Therefore it is important to know under what circumstances DNAPL penetrates low-permeability lenses.

In this paper we consider a porous medium containing a single low-permeable lens. DNAPL is released through an opening in the impermeable top boundary, and migrates down towards the lens. The objective of this paper is to show under what conditions DNAPL infiltrates into the lens. We give an explicit criterion for infiltration into the lens in terms of a critical DNAPL inflow rate. It will be obtained using simple analytical approximations that govern the qualitative flow behavior well.

Capillary forces play a main role in this problem, in particular the entry pressure of the lens and the corresponding threshold saturation. The entry pressure is the minimum capillary pressure that is needed for a nonwetting fluid (DNAPL) to enter a medium that is saturated by a wetting phase (water). A high entry pressure corresponds to a low-permeable medium. DNAPL arriving at the lens cannot immediately penetrate, because the capillary pressure is still smaller than the entry pressure of the lens. Hence DNAPL accumulates on top of the lens and spreads in response to lateral pressure gradients. It may happen that so much DNAPL accumulates on the lens that the capillary pressure exceeds the entry pressure: DNAPL then infiltrates into the lens.

We study the infiltration problem for lenses that are of greater extent than the width of the steady-state DNAPL plume in absence of the lens. Large lenses obstruct the flow such that distinct accumulation of DNAPL occurs on their top boundary. For small lenses we expect that the effect of accumulation is less, since DNAPL can relatively easily flow around. We consider only media with positive entry pressures.

The effect of capillary forces and heterogeneity is analyzed mathematically and numerically by Van Duijn et al. [6]. By a regularization procedure they derive the interface conditions needed at discontinuities in the permeability. Several authors study the problem of DNAPL infiltration numerically. Kueper and Frind [12,13] develop a finite difference model for two-phase flow in heterogeneous media and apply it to DNAPL infiltration problems. They perform sensitivity analyses for a geometry with a single lens, as well as for random permeability fields. However, they focus on the spreading of DNAPL caused by a low-permeable lens and consider only cases in which DNAPL penetrates the lens. Helmig [10] develops a numerical model based on the finite element method, and simulates the laboratory experiments by Kueper et al. [11].

This paper is organized as follows. In section 2 we state the model equations and the interface conditions used at the boundary of the lens, where the permeability is discontinuous. In section 3 we analyze the steady-state flow problem. Two configurations are studied: one without lens (homogeneous case), and one with a single lens (heterogeneous case). In the homogeneous case we derive an estimate for the width of the DNAPL plume as a function of depth. Further, we give an analytical solution for low DNAPL saturations. In the heterogeneous case we derive an explicit criterion that determines whether DNAPL infiltrates into the lens or not. In the analysis it is assumed that the DNAPL is in vertical equilibrium (VE) when it spreads laterally on top of the lens. We show that DNAPL infiltrates into the lens if a critical DNAPL discharge in the opening is exceeded. In the final section we present a numerical algorithm for the heterogeneous problem that incorporates the interface conditions. With this numerical scheme several simulations are carried out for a test problem. These computational results are in good agreement with the analytical results obtained in section 3.

2. Model equations

We consider the standard model for flow of two immiscible and incompressible fluids in a homogeneous porous medium. Let S_{w} denote the saturation of the wetting fluid and S_{n} the saturation of the nonwetting fluid,

$$S_{\mathrm{w}} + S_{\mathrm{n}} = 1. \tag{1}$$

Both phases satisfy the fluid-balance equations,

$$\phi \frac{\partial S_\alpha}{\partial t} + \operatorname{div} q_\alpha = 0, \quad \alpha = \mathrm{n}, \mathrm{w}, \tag{2}$$

where ϕ is the porosity of the porous medium and q_α the specific discharge of phase α. These specific discharges are given by Darcy's law,

$$q_\alpha = -\lambda_\alpha(\operatorname{grad} p_\alpha - \rho_\alpha g e_{\mathrm{g}}), \quad \alpha = \mathrm{n}, \mathrm{w}, \tag{3}$$

where λ_α, p_α and ρ_α are the mobility, pressure and density of phase α, g the acceleration of gravity, and e_{g} the unit-vector in the direction of gravity. The mobility of phase α is given by

$$\lambda_\alpha(S_\alpha) = k\frac{k_{\mathrm{r}\alpha}(S_\alpha)}{\mu_\alpha}, \quad \alpha = \mathrm{n}, \mathrm{w}, \tag{4}$$

where k is the absolute permeability of the porous medium, and $k_{\mathrm{r}\alpha}$ and μ_α the relative permeability and the viscosity of phase α. The total flow q_{t} of both phases is given by

$$q_{\mathrm{t}} = q_{\mathrm{w}} + q_{\mathrm{n}}. \tag{5}$$

Due to interfacial tension there is a pressure difference between the nonwetting and the wetting phase, which is called the capillary pressure p_{c},

$$p_{\mathrm{n}} - p_{\mathrm{w}} = p_{\mathrm{c}}(S_{\mathrm{w}}). \tag{6}$$

For a given rock type the capillary pressure p_{c} is a known function of the saturation.

In equations (1)–(6) we have four unknowns, S_α and p_α. Two of them are eliminated easily by using (1) and (6). Because we are interested in DNAPL flow, it is convenient to take the reduced DNAPL saturation s as one of the two dependent variables,

$$s = \frac{S_n - S_{nr}}{1 - S_{wr} - S_{nr}}, \tag{7}$$

where $S_{\alpha r}$ denotes the residual saturation of phase α. For the other dependent variable we take the wetting phase pressure p_w. This choice appears to be advantageous in the case of heterogeneities. If no confusion can arise, we drop the subscript w of p_w.

After some rearrangements the model equations are written as

$$\phi\frac{\partial s}{\partial t} + \operatorname{div} q_n = 0, \tag{8}$$

$$\operatorname{div} q_t = 0, \tag{9}$$

where

$$q_n = f_n q_t - \lambda_w f_n(\operatorname{grad} p_c - \Delta\rho g e_g), \tag{10}$$

$$q_t = -\lambda_n(\operatorname{grad} p_c - \Delta\rho g e_g) - (\lambda_w + \lambda_n)(\operatorname{grad} p_w - \rho_w g e_g), \tag{11}$$

and

$$f_n = \frac{\lambda_n}{\lambda_n + \lambda_w} \quad \text{and} \quad \Delta\rho = \rho_n - \rho_w.$$

The function f_n is called the fractional flow function of the nonwetting phase. In view of (4) it is a function of s only.

In this paper we restrict ourselves to capillary pressure curves with a nonzero capillary entry pressure p_e and an infinite capillary pressure at the residual water saturation,

$$p_c(s) = p_e J(s), \tag{12}$$

with

$$J(0) = 1 \quad \text{and} \quad J(1) = \infty, \tag{13}$$

where J is the rescaled J-Leverett function. For example, the Brooks and Corey model [2] features a nonzero entry pressure, whereas the Van Genuchten model [9] does not. According to the Leverett scaling [14] we have

$$p_e \propto \sigma\sqrt{\frac{\phi}{k}}, \tag{14}$$

where σ denotes the interfacial tension between the two fluids. We note that a lower permeability yields a higher entry pressure.

A nonzero entry pressure has interesting consequences if there are subdomains with different entry pressures. In each subdomain equations (8)–(11) apply. To connect the solutions in the different subdomains we use interface conditions.

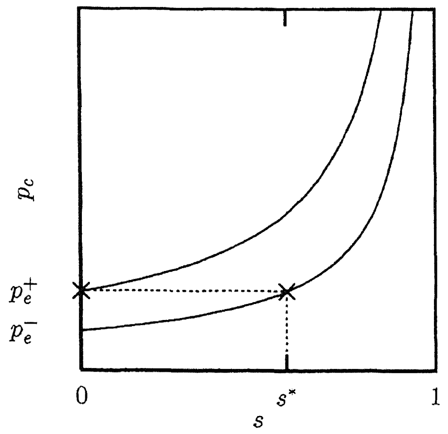

Figure 1. Capillary pressure p_c on both sides of an interface. If the entry pressures p_e are unequal, p_c cannot always be continuous.

The interface condition regarding the fluxes is immediate. Conservation of mass at the interface implies that the normal components of the fluxes q_n and q_t must be continuous across an interface.

The next interface condition involves the capillary pressure p_c. The boundedness of q_n and q_t in equations (10)–(11) implies that p_c and p_w should be continuous across an interface if both phases are mobile ($\lambda_w > 0$ and $\lambda_n > 0$). However, if the entry pressures are different on each side of the interface, a continuous capillary pressure is not always possible. This is illustrated by figure 1. Figure 1 shows two capillary pressure curves for different entry pressures p_e^- and p_e^+, where $p_e^+ > p_e^-$. Let s^- denote the saturation on the side with lowest entry pressure, and s^+ the saturation on the other side. The capillary pressure cannot be continuous at the interface if s^- is below the threshold saturation s^*,

$$J(s^*) = \frac{p_e^+}{p_e^-}. \tag{15}$$

This problem has been analyzed by Van Duijn et al. [6] for a one-dimensional flow without gravity. A similar analysis for a line normal to the interface gives the following *extended capillary pressure condition.* If $s^- \geqslant s^*$ the capillary pressure must be continuous. However, if $s^- < s^*$ the capillary pressure is discontinuous, and s^+ must be zero. A consequence of this condition is that DNAPL can enter a region with higher entry pressure only if its saturation exceeds the threshold saturation s^*.

The last interface condition concerns the water pressure p_w. Because the capillary pressure can be discontinuous, we have in view of (6) that p_w and p_n (or both) may be discontinuous. It follows from the extended capillary pressure condition that the capillary pressure is only discontinuous if $s^- < s^*$ and $s^+ = 0$. However, the boundedness of q_w in (3) implies that p_w can only be discontinuous if $s^- = 1$ or

$s^+ = 1$. Therefore p_w must be continuous, even if p_c is discontinuous. Hence p_n is discontinuous whenever p_c is discontinuous.

Summarizing, we have the following interface conditions for the situation shown in figure 1:

- $n \cdot q_n$ and $n \cdot q_t$ are continuous, where n denotes the unit vector normal to the interface,
- the extended capillary pressure condition,

$$\begin{cases} p_c^+(s^+) = p_c^-(s^-), & \text{if } s^- \geqslant s^*, \\ s^+ = 0, & \text{if } s^- < s^*, \end{cases} \tag{16}$$

- p_w is continuous.

3. Analysis of steady-state DNAPL flow

In this section we consider two-dimensional steady-state flow of DNAPL for two configurations: (i) a homogeneous porous medium, and (ii) a homogeneous host medium containing a horizontal lens with a higher entry pressure. In both cases the flow takes place in a semi-infinite domain, as depicted in figure 2. The DNAPL sinks through an opening in the impermeable top boundary into the domain. Gravity is directed vertically downward. In the heterogeneous case the lens is located symmetrically beneath the opening.

For the homogeneous problem we aim at finding an estimate of the DNAPL plume width as a function of depth. The objective for the heterogeneous problem is to find a criterion that can be used to determine whether DNAPL infiltrates into the lens or not. In the analysis of the latter problem we assume that the length of the lens is much greater than the width of the steady-state DNAPL plume for the configuration without a lens. In that case we expect that DNAPL is forced to flow laterally on the lens. The condition on the length of the lens can be checked with the estimate for the plume width.

To arrive at problems which can be treated analytically, we make a few approximations. For both the homogeneous and heterogeneous case we assume that the total

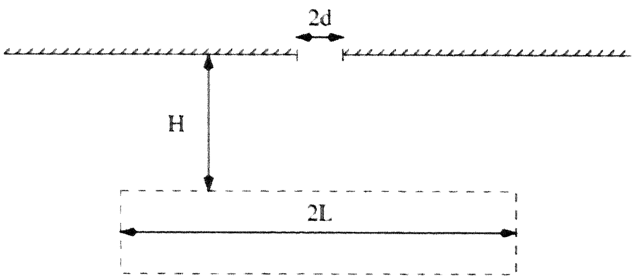

Figure 2. Geometry of configuration with a single lens.

flow is small with respect to the other terms in (10), so that it can be disregarded. The system of two coupled equations (8)–(9) then reduces to a single equation for the DNAPL saturation. Within this approximation, the flow is counter-current: the specific discharge of water is directed oppositely to the specific discharge of DNAPL in every point of the domain. In section 3.3 we show that this approximation is reasonable if the DNAPL saturation is sufficiently low.

In the homogeneous case we assume moreover that the flow in the vertical direction due to capillary pressure gradients can be disregarded compared with the flow caused by density differences. In the heterogeneous case we assume that the laterally spreading DNAPL on top of the lens is in vertical equilibrium (VE), and that it drops off of the lens so quickly that the saturation at both ends is approximately zero. VE means that the buoyancy force (caused by density differences) is balanced by the capillary force, so that the DNAPL flow in the vertical direction can be disregarded.

For the analysis in this section we need the properties of the functions $k_{\mathrm{r}\alpha}$ and J. It is assumed that k_{rw} and k_{rn} are continuously differentiable on $[0,1]$, that J is continuously differentiable on $[0,1)$ with derivative J', and that they satisfy:

- $k_{\mathrm{rn}}(s)$ is strictly increasing with $k_{\mathrm{rn}}(0) = 0$,
- $k_{\mathrm{rw}}(s)$ is strictly decreasing with $k_{\mathrm{rw}}(1) = 0$,
- $J'(s) > 0$ on $(0,1)$, $J(0) = 1$ and $J(1) = \infty$,
- $J'(s)k_{\mathrm{rw}}(s)k_{\mathrm{rn}}(s)$ is continuous on $[0,1]$.

For example, the functions of the Brooks–Corey model satisfy the above hypotheses.

3.1. Steady-state infiltration in a homogeneous medium

In this section we consider the steady-state infiltration of DNAPL in a semi-infinite domain, $\Omega = \mathbb{R} \times (0,\infty)$. The coordinate in the vertical downward direction is denoted by z. Both the entry pressure and the absolute permeability of the porous medium are constant in Ω.

Using the approximation $q_{\mathrm{t}} = 0$ we obtain from equations (8)–(11) for a steady-state flow

$$\operatorname{div} q_{\mathrm{n}} = 0, \qquad q_{\mathrm{n}} = -\lambda_{\mathrm{w}} f_{\mathrm{n}} \operatorname{grad}(p_{\mathrm{c}} - \Delta\rho g z) \quad \text{in } \Omega. \tag{17}$$

The DNAPL enters the domain through an opening of width $2d$ in the impermeable top boundary at $z = 0$,

$$n \cdot q_{\mathrm{n}}(x,0) = \begin{cases} -q_{\mathrm{n}}^{\mathrm{i}}, & \text{if } |x| \leqslant d, \\ 0, & \text{if } |x| > d, \end{cases} \tag{18}$$

where n is the outwards directed normal of the top boundary. We seek a solution $s = s(x,z)$ of the above problem which vanishes as $\|x\| \to \infty$.

To simplify the above problem, we use the assumption that the force induced by the density difference is dominant compared with the capillary force in the vertical direction,

$$\frac{1}{\Delta\rho g}\left|\frac{\partial p_{\rm c}}{\partial z}\right| \ll 1 \quad \text{in } \Omega. \tag{19}$$

This is often a reasonable approximation for media with high permeability. Disregarding the capillary gradient term in the vertical direction in (17)–(18) yields

$$\Delta\rho g\frac{\partial}{\partial z}(f_{\rm n}\lambda_{\rm w}) = \frac{\partial}{\partial x}\left(f_{\rm n}\lambda_{\rm w}\frac{\partial p_{\rm c}}{\partial x}\right), \tag{20}$$

with the boundary condition at $z = 0$:

$$\Delta\rho g f_{\rm n}\lambda_{\rm w} = \begin{cases} q_{\rm n}^{\rm i}, & \text{if } |x| \leqslant d, \\ 0, & \text{if } |x| > d. \end{cases} \tag{21}$$

We note that condition (21) only makes sense if $q_{\rm n}^{\rm i}$ is smaller than the maximum value of $\Delta\rho g f_{\rm n}(s)\lambda_{\rm w}(s)$. Equations (20)–(21) serve as a starting point for the analysis of the homogeneous configuration.

To write the equations in dimensionless form, we redefine x and z according to

$$x := \frac{x}{d}, \qquad z := \frac{z}{d},$$

and define the dimensionless numbers

$$N_{\rm cg} = \frac{p_{\rm e}}{\Delta\rho g d}, \qquad N_q = \frac{q_{\rm n}^{\rm i}\mu_{\rm n}}{k\Delta\rho g}, \qquad M = \frac{\mu_{\rm n}}{\mu_{\rm w}}. \tag{22}$$

The number $N_{\rm cg}$ represents the ratio of capillary force and buoyancy force, N_q the rescaled inflow, and M the mobility ratio. From (20) and (12) we obtain

$$\frac{\partial}{\partial z}\bar{\lambda}(s) = N_{\rm cg}\frac{\partial}{\partial x}\left(D(s)\frac{\partial s}{\partial x}\right), \tag{23}$$

where

$$\bar{\lambda}(s) = \frac{k_{\rm rw}(s)k_{\rm rn}(s)}{k_{\rm rw}(s) + k_{\rm rn}(s)/M} \quad \text{and} \quad D(s) = J'(s)\bar{\lambda}(s). \tag{24}$$

The boundary condition at $z = 0$ is written as

$$\bar{\lambda}\big(s(x,0)\big) = v_0(x) = \begin{cases} N_q, & \text{if } |x| \leqslant 1, \\ 0, & \text{if } |x| > 1. \end{cases} \tag{25}$$

As mentioned earlier, it is necessary that N_q is less than the maximum value of $\bar{\lambda}(s)$ on $[0, 1]$. Note that this is a consequence of approximation (19). Let $\bar{s}$ denote the maximum value such that $\bar{\lambda}' > 0$ on $(0, \bar{s})$, as shown in figure 3. For most models found in the literature (e.g., the Brooks–Corey model) $\bar{s}$ coincides with the value at which $\bar{\lambda}$ attains its maximum on $[0, 1]$. We only consider the case that $N_q < \bar{\lambda}(\bar{s})$.

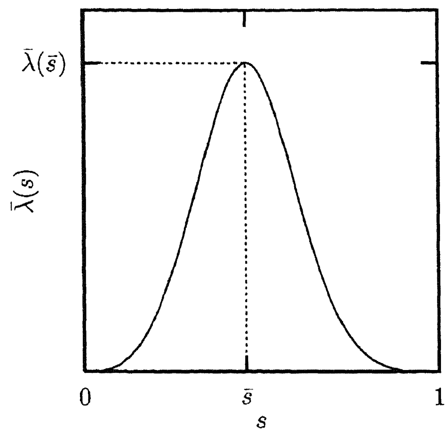

Figure 3. Choice of $\bar{s}$: $\bar{\lambda}(s)$ is invertible on $[0, \bar{s}]$.

3.1.1. Estimate of the DNAPL plume width

We rewrite equation (23) so that it can be recognized as an equation of diffusion type. To that end we define $v = v(x, z)$ as

$$v = \bar{\lambda}(s). \tag{26}$$

Since $\bar{\lambda}(s)$ is strictly increasing on $[0, \bar{s}]$, it is invertible. Let $\bar{\lambda}^{-1}$ denote its inverse, defined on $[0, \bar{v}]$ with $\bar{v} = \bar{\lambda}(\bar{s})$. Then we obtain from equations (23)–(25) the following problem for v:

$$\text{(I)} \quad \begin{cases} \dfrac{\partial v}{\partial z} = N_{\text{cg}} \dfrac{\partial}{\partial x}\left(\widetilde{D}(v)\dfrac{\partial v}{\partial x}\right), & -\infty < x < \infty,\ z > 0, \\ v(x, 0) = v_0(x), & -\infty < x < \infty, \end{cases}$$

where

$$\widetilde{D}(v) = \frac{D(\bar{\lambda}^{-1}(v))}{\bar{\lambda}'(\bar{\lambda}^{-1}(v))} \quad \text{for } 0 < v < \bar{v}. \tag{27}$$

To keep the presentation clear and simple, we confine ourselves to functions $\widetilde{D}$ that are continuous on $[0, \bar{v})$. This is the case, for example, when $\bar{\lambda}'$ behaves as a power function near $s = 0$.

Problem (I) can be recognized as a nonlinear diffusion problem when z is viewed as the time coordinate. The problem is called degenerate parabolic if $\widetilde{D}(0) = 0$. A feature of degenerate parabolic problems is that free boundaries may occur. In the (x, z)-plane they correspond to the boundaries separating the region where DNAPL is present ($v > 0$) from the region containing only water ($v = 0$). They constitute the boundary of the infiltrating DNAPL plume. For general $\widetilde{D}$ we cannot obtain a closed-form solution for this problem. Fortunately, with the use of a comparison principle we can estimate the width of the DNAPL plume.

The comparison principle for problem (I) is as follows (see, e.g., [16,19]). Let $v_0^1(x)$ and $v_0^2(x)$ denote two functions in the boundary condition at $z = 0$ satisfying $v_0^1(x) \leqslant v_0^2(x)$ on $\mathbb{R}$. The corresponding solutions then satisfy $v^1(x,z) \leqslant v^2(x,z)$ in Ω. Since $v \equiv N_q$ is a solution of the differential equation of problem (I) corresponding to the conditions $v_0 \equiv N_q$, it immediately follows from the comparison principle that the solution of problem (I) satisfies $v \leqslant N_q$. By taking $N_q < \bar{v}$ we establish that $v(x,z) < \bar{v}$ in Ω. Equally, one can show $v(x,z) \geqslant 0$ in Ω.

To estimate the width of the DNAPL plume, we compare the solution of problem (I) with the self-similar solution $V(x,z)$ corresponding to the following boundary condition at $z = 0$:

$$V(x,0) = \begin{cases} N_q, & \text{if } x \leqslant 1, \\ 0, & \text{if } x > 1, \end{cases} \tag{28}$$

so that $v_0(x) \leqslant V(x,0)$ (see (25)). Hence by the comparison principle it follows that $v(x,z) \leqslant V(x,z)$ in Ω. The similarity solution V is obtained by using the similarity transformation

$$V(x,z) = g(\eta), \quad \text{where } \eta = \frac{x-1}{\sqrt{z}}.$$

Then g satisfies

$$\begin{cases} \frac{1}{2}\eta g' + N_{\mathrm{cg}}\big(\widetilde{D}(g)g'\big)' = 0, & -\infty < \eta < \infty, \\ g(-\infty) = N_q \quad \text{and} \quad g(\infty) = 0, \end{cases}$$

where primes denote differentiation with respect to η. Van Duijn and Peletier [7] show that this problem has a unique solution.

If $\widetilde{D}(0) = 0$ there may exist a number a_{n} such that g vanishes identically for $\eta \geqslant a_{\mathrm{n}}$, and that g is positive on $(0, a_{\mathrm{n}})$. In the (x,z)-plane this situation corresponds to a free boundary $x = 1 + a_{\mathrm{n}}\sqrt{z}$, which separates the region $V > 0$ from $V = 0$. In [7] a condition is given for the existence of this finite number a_{n}: it exists if and only if

$$\int_0^{N_q} \frac{\widetilde{D}(g)}{g}\,\mathrm{d}g < \infty. \tag{29}$$

This condition is satisfied because

$$I_1 = \int_0^{N_q} \frac{\widetilde{D}(g)}{g}\,\mathrm{d}g = \int_0^{\bar{\lambda}^{-1}(N_q)} \frac{D(s)}{\bar{\lambda}(s)}\,\mathrm{d}s = J\big(\bar{\lambda}^{-1}(N_q)\big) - 1 < \infty. \tag{30}$$

Thus a free boundary exists separating the region $V = 0$ from $V > 0$. From (30) we also have that $\widetilde{D}(0) = 0$.

Since the solution v of problem (I) has to be nonnegative, it follows from the comparison principle that v is identical to zero for $x \geqslant 1 + a_{\mathrm{n}}\sqrt{z}$. By symmetry we have that v vanishes for $|x| \geqslant 1 + a_{\mathrm{n}}\sqrt{z}$. In [1] it is shown that the number a_{n} is bounded by $\bar{a} = 2\sqrt{N_{\rm cg} I_1}$. Let $f(z)$ denote the half of the width of the DNAPL plume as a function of depth, then we have

$$f(z) \leqslant 1 + \bar{a}\sqrt{z}, \quad \text{where } \bar{a} = 2\sqrt{N_{\rm cg}\left[J\left(\bar{\lambda}^{-1}(N_q)\right) - 1\right]}. \tag{31}$$

This estimate is not sharp: it overestimates the width in general. For small saturations, however, we can also obtain an asymptotic expression for the plume width.

3.1.2. Asymptotic solution for small saturations

Here we consider a special case for which an explicit solution is known, namely when $\widetilde{D}(v)$ is a power function. In general it is not, but for small values of v we can often approximate $\widetilde{D}(v)$ by

$$\widetilde{D}(v) \sim Cv^p \quad \text{as } v \downarrow 0, \tag{32}$$

where $C > 0$ and $p > 0$. When we substitute this in problem (I) we obtain

$$\frac{\partial v}{\partial z} = C N_{\rm cg} \frac{\partial}{\partial x}\left(v^p \frac{\partial v}{\partial x}\right) \quad \text{in } \Omega. \tag{33}$$

This nonlinear diffusion equation is known in the mathematical literature as the porous media equation. For an overview of the mathematical results concerning equation (33) we refer the reader to [18,20]. The point-source solution of equation (33), the Barenblatt–Pattle solution, has the form

$$v(x,z) = \frac{A}{f(z)}\left(1 - \frac{x^2}{f(z)^2}\right)_+^{1/p}, \tag{34}$$

where

$$f(z) = \left(1 + \frac{2(p+2)}{p} A^p C N_{\rm cg}\, z\right)^{1/(p+2)}, \tag{35}$$

and $(\cdot)_+ = \max(0, \cdot)$. We choose the parameter A such that the total discharge through the opening is equal to $2N_q$ (see (25)),

$$\int_{-\infty}^{\infty} v(x,0)\,\mathrm{d}x = \int_{-\infty}^{\infty} A\left(1 - x^2\right)_+^{1/p} \mathrm{d}x = 2N_q. \tag{36}$$

We mention that a similar approach to obtain an asymptotic solution is found in [5] for the case of an air sparging problem.

An explicit expression for the curves representing constant saturation levels is easily obtained from (26) and (34). The boundary of the Barenblatt–Pattle solution is given by $|x| = f(z)$. We observe that the corresponding DNAPL plume is narrower for smaller values of A, i.e., for smaller discharges through the opening.

We remark that (34) is the asymptotic solution of equation (33) subject to the original boundary condition (25), for large values of z (see [8]). From (35) we observe that $f(z) = \mathcal{O}(z^{1/(p+2)})$ for large values of z. This is in agreement with the estimate (31) for the width of the plume, because $p > 0$.

3.2. DNAPL infiltration into a lens with high entry pressure

In this section we consider the steady-state flow of DNAPL and water in a domain containing a single horizontal lens. The entry pressure of the lens p_e^l is greater than the entry pressure of the host medium p_e^h. We want to determine the conditions for which a steady-state solution is possible such that DNAPL does not infiltrate into the lens. The DNAPL saturation on the lens boundary must then be smaller than the threshold saturation s^*.

The configuration is depicted in figure 2. The upper boundary of the lens is located at a depth H with respect to the top boundary of the domain and the length of the lens is $2L$. The normal component of the DNAPL discharge on the top boundary is prescribed by (18). The configuration is symmetrical with respect to $x = 0$; therefore we only consider the right half of the domain.

To obtain a problem that can be treated analytically we have to make some simplifications. The validity of the simplifications will be verified by numerical experiments.

As for the homogeneous case we assume that the total flow q_t is so small that it can be disregarded; this is reasonable for small DNAPL saturations. Furthermore, we assume that the DNAPL flow on top of the lens is mainly horizontal towards the sides. We expect that this is the case when the lens is much longer than the steady-state DNAPL plume width at $z = H$ corresponding to a homogeneous configuration without lens. The plume width can be estimated with the use of (31) or (35).

In this section we restrict the analysis to the horizontal flow on top of the lens. The situation is shown schematically in figure 4. The discharge of DNAPL transported

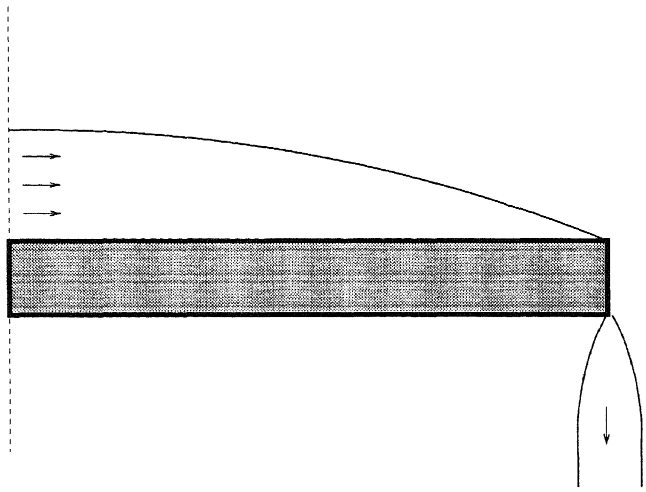

Figure 4. Flow of DNAPL over lens.

over the lens to the right end is equal to half the discharge of supplied DNAPL in the opening of the top boundary of the domain. We assume that the flow on top of the lens is in vertical equilibrium. It means that the flow in vertical direction can be disregarded compared with the flow in horizontal direction, which yields

$$\frac{\partial p_c}{\partial z} = \Delta \rho g \quad \text{if } 0 < s < 1. \tag{37}$$

Moreover, we assume that the DNAPL drops off at the end of the lens so quickly that the saturation there is approximately zero, i.e., $s(x, H)$ is positive for $x < L$ and $s(x, H) \to 0$ as $x \to L$.

After integration of the horizontal component of q_n as given in (17) with respect to the height, we obtain

$$\frac{Q_i}{2} = -\int_0^H \lambda_w f_n \frac{\partial p_c}{\partial x} \, dz \quad \text{for } 0 \leqslant x \leqslant L, \tag{38}$$

where $Q_i = 2dq_n^i$. To put equations (37) and (38) in dimensionless form we redefine x and z as

$$x := \frac{x}{L} \quad \text{and} \quad z := \frac{z}{H},$$

and define the dimensionless numbers

$$N_c = \frac{2p_e^h k_h H}{L\mu_n Q_i} \quad \text{and} \quad N_{cg} = \frac{p_e^h}{\Delta \rho g H}. \tag{39}$$

The number N_c is the capillary number, which represents the ratio of capillary and viscous forces in the horizontal direction. Note that the top boundary of the lens is located at $z = 1$. Writing (37) and (38) in dimensionless form we obtain

$$-N_c \int_0^1 \bar{\lambda}(s) \frac{\partial}{\partial x} J(s) \, dz = 1, \quad 0 \leqslant x \leqslant 1, \tag{40}$$

and

$$N_{cg} \frac{\partial}{\partial z} J(s) = 1 \quad \text{if } 0 < s < 1. \tag{41}$$

We seek a solution $s(x, z)$ of equations (40)–(41) that satisfies $0 < s(x, 1) \leqslant s^*$ for $x < 1$ and $s(1, 1) = 0$.

Let $s_b(x)$ denote the DNAPL saturation on the lens boundary $z = 1$. From (41) we then obtain

$$J\big(s(x, z)\big) = J\big(s_b(x)\big) - \frac{1 - z}{N_{cg}}. \tag{42}$$

Hence, if we would know the saturation $s_b(x)$ on the lens boundary then the saturation distribution $s(x, z)$ above the lens is given by (42). To find s_b we substitute (42) into

(40) and rewrite (40) as an ordinary differential equation for s_b. Differentiating (42) with respect to x gives

$$\frac{\partial}{\partial x} J\big(s(x,z)\big) = \frac{\mathrm{d}}{\mathrm{d}x} J\big(s_\mathrm{b}(x)\big). \tag{43}$$

The integrand in (40) vanishes when $s = 0$, because $\bar{\lambda}(0) = 0$. From (42) we find that no DNAPL is present for values of z satisfying

$$z < 1 - N_\mathrm{cg}\big(J\big(s_\mathrm{b}(x)\big) - 1\big) := z_0(x). \tag{44}$$

Using (42)–(44) we obtain from (40) the following problem for s_b:

$$\text{(II)} \quad \begin{cases} -N_\mathrm{c}\langle D\rangle(s_\mathrm{b})\dfrac{\mathrm{d}s_\mathrm{b}}{\mathrm{d}x} = 1 & \text{for } 0 \leqslant x < 1, \\ s_\mathrm{b}(1) = 0, \end{cases}$$

where $\langle D\rangle$, which can be interpreted as an effective vertically averaged diffusion function (cf. (24)), is given by

$$\langle D\rangle(s_\mathrm{b}) = J'(s_\mathrm{b}) \int_{z_0}^{1} \bar{\lambda}\big(s(x,z)\big)\,\mathrm{d}z = N_\mathrm{cg} J'(s_\mathrm{b}) \int_0^{s_\mathrm{b}} D(s)\,\mathrm{d}s, \tag{45}$$

where $s(x,z)$ is given by (42), z_0 by (44), and $D(s) = J'(s)\bar{\lambda}(s)$. We note that $\langle D\rangle(0) = 0$ and $\langle D\rangle(s_\mathrm{b}) > 0$ for $s_\mathrm{b} > 0$. Hence it follows from the differential equation that $s_\mathrm{b}(x)$ is strictly decreasing if $s_\mathrm{b} > 0$. Integration of the differential equation for s_b yields the implicit solution

$$N_\mathrm{c} \int_0^{s_\mathrm{b}(x)} \langle D\rangle(u)\,\mathrm{d}u = 1 - x, \quad 0 \leqslant x \leqslant 1. \tag{46}$$

Using (45) we can simplify this expression to

$$N_\mathrm{c} N_\mathrm{cg} I\big(s_\mathrm{b}(x)\big) = 1 - x, \quad 0 \leqslant x \leqslant 1, \tag{47}$$

where

$$I(s_\mathrm{b}) = \int_0^{s_\mathrm{b}} \left(J'(u) \int_0^{u} D(s)\,\mathrm{d}s\right)\mathrm{d}u = \int_0^{s_\mathrm{b}} \big[J(s_\mathrm{b}) - J(s)\big] D(s)\,\mathrm{d}s. \tag{48}$$

Note that I is a strictly increasing function of s_b with $I(0) = 0$. A closed-form expression for the curves corresponding to constant saturation levels is given by (42), (47) and (48).

If $s_\mathrm{b}(x) \leqslant s^*$, DNAPL does not flow into the lens. Since $s_\mathrm{b}(x)$ is strictly decreasing, we need $s_\mathrm{b}(0) \leqslant s^*$, or equivalently $N_\mathrm{c} N_\mathrm{cg} I(s^*) \geqslant 1$. Substituting the expressions for the dimensionless numbers (39) into the latter inequality, we find that $s_\mathrm{b} \leqslant s^*$ provided that

$$Q_\mathrm{i} \leqslant Q_\mathrm{i}^* = \frac{2k_\mathrm{h}(p_\mathrm{e}^\mathrm{h})^2}{\mu_\mathrm{n}\Delta\rho g L} I(s^*), \tag{49}$$

where Q_i^* is the critical discharge. Thus if $Q_i > Q_i^*$, there is no steady-state solution for which s is smaller than s^* on the entire lens boundary, and consequently DNAPL infiltrates into the lens. We remark that this criterion does not depend explicitly on the depth H of the lens.

Clearly, the critical discharge derived here is not exact, but should be considered as an estimate of its magnitude. The quality of this estimate and the corresponding criterion (49) will be checked in section 4.2, where we consider the time-dependent solution for drainage of initially water-saturated media. If the total flow is zero, and the steady-state solution does not penetrate the lens, then the time-dependent solution is bounded for all times by the steady-state solution. This implies that also for the time-dependent problem DNAPL does not infiltrate into the lens if $Q_i \leqslant Q_i^*$.

3.3. *Motivation of the approximation $q_t \equiv 0$*

In both the homogeneous and heterogeneous case we have assumed that the total flow q_t is so small that it can be disregarded. Here we show that with certain natural boundary conditions at infinity this is a reasonable approximation for the homogeneous case if

$$\frac{\Delta\rho}{\rho_w} f_n(s) \ll 1. \tag{50}$$

Observe that (50) is satisfied for sufficiently low DNAPL saturations.

The exact steady-state flow problem is governed by equations (8)–(11) with $\partial s/\partial t \equiv 0$. At the top boundary of the domain let $n \cdot q_n$ be given by (18) and $n \cdot q_t = 0$. The amount of DNAPL entering is equal to the amount of water leaving through the opening. Let $\psi_w = p_w - \rho_w g z$ denote the water potential. At infinity, the DNAPL saturation vanishes and the water pressure becomes hydrostatic. Therefore we prescribe the following conditions at infinity:

$$s \to 0, \quad \psi_w \to 0 \quad \text{as } \|x\| \to \infty. \tag{51}$$

To prevent flow at infinity we seek solutions of (8) and (9) for which $\|q_t\| = \mathcal{O}(\|x\|^{-1})$ as $\|x\| \to \infty$. To show the structure of q_t we rewrite expression (11) as

$$q_t = -\lambda_t(s)\,\mathrm{grad}\,P + \left(1 + \frac{\Delta\rho}{\rho_w} f_n(s)\right)\lambda_t(s)\,\mathrm{grad}\,\rho_w g z,$$

where $\lambda_t = \lambda_w + \lambda_n$, and P the global pressure (see, e.g., [3]) defined by

$$P = \int_0^s f_n(u)p_c'(u)\,\mathrm{d}u + p_w. \tag{52}$$

Then, using (50) we find for q_t

$$q_t \approx -\lambda_t(s)\,\mathrm{grad}\,\psi_t, \quad \text{where } \psi_t = P - \rho_w g z. \tag{53}$$

From (51) and (52) it follows that $\psi_t \to 0$ as $\|x\| \to \infty$.

Let us define

$$\Omega_R = \{(x,z) \in \Omega\colon\ x^2 + z^2 < R^2\}.$$

The boundary of Ω_R is denoted by $\partial\Omega_R$. When we multiply (9) by ψ_t and integrate over Ω_R, we find

$$\int_{\Omega_R} \operatorname{grad}\psi_t \cdot q_t = \int_{\partial\Omega_R} (n \cdot q_t)\psi_t, \tag{54}$$

where n denotes the outwards directed normal at the boundary $\partial\Omega_R$. The right-hand side of (54) vanishes for $R \to \infty$ in view of the boundary condition at $z = 0$ and the behavior of q_t and ψ_t at infinity. Then letting $R \to \infty$ in (54) we obtain after substitution of (53)

$$\int_\Omega \lambda_t \|\operatorname{grad}\psi_t\|^2 = 0.$$

Since λ_t is bounded away from zero, it follows that $\|\operatorname{grad}\psi_t\| = 0$ in Ω. Hence for the approximated total flow rate (53) we obtain $q_t = 0$ in Ω. Note that approximation (53) and the corresponding result $q_t \equiv 0$ is exact if $\Delta\rho = 0$.

The result that $q_t = 0$ in Ω can also be obtained for a different boundary condition at the top boundary $z = 0$, which may seem more realistic. If we prescribe in the opening $s > 0$ and $n \cdot q_t = 0$, and along the remaining part $s = 0$ and $p_w = 0$, then we have along the top boundary either $n \cdot q_t = 0$ or $\psi_t = 0$. The contribution of the integral along the top boundary in (54) vanishes in that case as well, yielding the same result.

The argument given here cannot be applied directly to the heterogeneous configuration, because ψ_t is in general not continuous across the lens boundary. However, if we assume that $n \cdot q_t = 0$ on the lens boundary it can be concluded that $q_t = 0$ in the entire domain.

4. Numerical approach

4.1. Discretization

In this section we present a numerical algorithm, in which the interface conditions as discussed in section 2 are explicitly incorporated. Because the capillary pressure may be discontinuous across an interface, a careful discretization near the lens boundary is needed. In [6] we have developed a similar discretization for one-dimensional problems. Here we present the two-dimensional extension of this algorithm.

For the discretization of equations (1)–(6) we use the standard fully-implicit scheme (see, e.g., [17]) on a Cartesian grid, with the reduced DNAPL saturation s and the water pressure p as the independent variables. For ease of notation we consider a constant mesh size h. We assume that the lens is resolved by the grid. Integration of the conservation laws (2) over the cell (i,j) yields

$$-\frac{\phi}{\Delta t}\left(s_{i,j}^{m+1}-s_{i,j}^{m}\right)+\frac{1}{h}\left(q_{\mathrm{w};i+1/2,j}^{m+1}-q_{\mathrm{w};i-1/2,j}^{m+1}+q_{\mathrm{w};i,j+1/2}^{m+1}-q_{\mathrm{w};i,j-1/2}^{m+1}\right)=0, \quad (55)$$

$$+\frac{\phi}{\Delta t}\left(s_{i,j}^{m+1}-s_{i,j}^{m}\right)+\frac{1}{h}\left(q_{\mathrm{n};i+1/2,j}^{m+1}-q_{\mathrm{n};i-1/2,j}^{m+1}+q_{\mathrm{n};i,j+1/2}^{m+1}-q_{\mathrm{n};i,j-1/2}^{m+1}\right)=0, \quad (56)$$

where the subscript (i,j) denotes the discretization cell, the superscript m the time, and $q_{\alpha;i+1/2,j}^{m+1}$ the approximation of the flux q_α at the edge between the cells (i,j) and $(i+1,j)$. The use of the backward Euler scheme in equations (55)–(56) guarantees the stability of the time integration scheme. The flux $q_{\alpha;i+1/2,j}$ is approximated in the usual way,

$$q_{\alpha;i+1/2,j}(s_{i,j},p_{i,j};s_{i+1,j},p_{i+1,j})=-\lambda_{\alpha;i+1/2,j}\Phi_{\alpha;i+1/2,j}, \quad \alpha=\mathrm{n},\mathrm{w}, \quad (57)$$

where

$$\Phi_{\mathrm{w};i+1/2,j}=\frac{1}{h}(p_{i+1,j}-p_{i,j})-\rho_{\mathrm{w}}g e_{\mathrm{g},1},$$
$$\Phi_{\mathrm{n};i+1/2,j}=\frac{1}{h}(p_{i+1,j}+p_{\mathrm{c};i+1,j}-p_{i,j}-p_{\mathrm{c};i,j})-\rho_{\mathrm{n}}g e_{\mathrm{g},1},$$

$e_{\mathrm{g},1}$ the component of e_{g} in the first coordinate direction, and $\lambda_{\alpha;i+1/2,j}$ the upwind weighted phase mobility,

$$\lambda_{\alpha;i+1/2,j}=\begin{cases} kk_{\mathrm{r}\alpha}(s_{i,j})/\mu_\alpha, & \text{if } \Phi_{\alpha;i+1/2,j}\leqslant 0,\\ kk_{\mathrm{r}\alpha}(s_{i+1,j})/\mu_\alpha, & \text{if } \Phi_{\alpha;i+1/2,j}>0. \end{cases} \quad (58)$$

We are now ready to define the discretization of $q_{\alpha;i+1/2,j}$ at the lens boundary. Because the saturation s is discontinuous, we introduce *dummy* variables s^{l} and s^{r} that can be considered as approximations of the left and right limit values of s at the interface (see also [4]). Further we introduce the dummy variable p^{m} which is an approximation of the continuous water pressure p at the interface. Using equation (57) and the dummy variables s^{l}, s^{r}, p^{m} we define approximations q_α^{l} and q_α^{r} to the flux $q_{\alpha;i+1/2,j}$ inside the cells (i,j) and $(i+1,j)$. Next, the dummy variables are eliminated by using continuity of flux,

$$q_\alpha^{\mathrm{l}}\left(s_{i,j},p_{i,j};s^{\mathrm{l}},p^{\mathrm{m}}\right)=q_\alpha^{\mathrm{r}}\left(s^{\mathrm{r}},p^{\mathrm{m}};s_{i+1,j},p_{i+1,j}\right), \quad \alpha=\mathrm{n},\mathrm{w}, \quad (59)$$

and the extended capillary pressure condition (16) for s^{l} and s^{r}. This system of three nonlinear equations is solved by Newton's method. Thus we obtain s^{l}, s^{r}, p^{m}, and the desired approximation to the flux:

$$q_{\alpha;i+1/2,j}=q_\alpha^{\mathrm{l}}=q_\alpha^{\mathrm{r}}. \quad (60)$$

The time step Δt^n is chosen adaptively, such that the changes in the saturation are of order $\Delta\bar{s}$,

$$\Delta t^{n+1} = \frac{\Delta\bar{s}}{\max_{i,j} |s^n_{i,j} - s^{n-1}_{i,j}|}\Delta t^n. \tag{61}$$

The ratio $\Delta t^{n+1}/\Delta t^n$ is bounded between 0.5 and 2.0, and in our actual computations we take $\Delta\bar{s} = 0.05$.

In every time step we have to solve the system of nonlinear equations (55)–(56), which is done by Newton's method. In the linearization we need the derivatives of $q_{\alpha;i+1/2,j}$ with respect to the independent variables in the adjacent cells. At heterogeneities the calculation of these derivatives is not trivial. However, a simple but tedious calculation shows that the dummy variables s^{l}, s^{r} and p^{m} can be eliminated from these derivatives. Therefore the linear system to be solved retains its usual sparsity pattern. The linear system is solved efficiently by means of a multigrid method (see [15]).

4.2. Computational results

We now use this algorithm to compare the numerical solution with the approximations derived in section 3. We consider both the spreading of a DNAPL plume in a homogeneous medium, and the infiltration of DNAPL in a laboratory set-up with a single lens. The relative permeabilities and capillary pressure functions are given by the Brooks–Corey model:

$$J(s) = (1-s)^{-1/\lambda} \tag{62}$$

and

$$k_{\mathrm{rn}}(s) = s^2\left(1-(1-s)^{1+2/\lambda}\right), \qquad k_{\mathrm{rw}}(s) = (1-s)^{3+2/\lambda}. \tag{63}$$

The value for λ is given in table 1 together with other relevant parameter values. These data are essentially taken from a study by Kueper et al. [13] and have been slightly modified for our purposes.

4.2.1. Steady-state DNAPL flow in a homogeneous medium

In section 3.1 we considered the steady-state infiltration of DNAPL in a homogeneous porous medium. An approximation of the saturation profile was derived under the assumption that the DNAPL saturation is small. For the Brooks–Corey model we have the small saturation approximation (32) with $p = 1/3$ and $C = (p/\lambda)[\lambda/(2+\lambda)]^p$. Figure 5 shows the quality of the small saturation approximation for $\lambda = 2.48$.

Let us now compare the explicit solution (34) of the porous media equation with the numerical solution for the data given in table 1. DNAPL infiltrates through the opening of width $2d$ with a rate $q^{\mathrm{i}}_{\mathrm{n}} = 1.35 \times 10^{-7}\,\mathrm{ms}^{-1}$. This is the largest flow rate that we consider in the next section, thus the case with the largest spreading of the DNAPL plume (cf. section 3.1).

Table 1
Data set of parameters used in numerical simulation.

Parameter	Value	Meaning
ϕ	0.34	porosity
k_h	$7.0 \times 10^{-12}\,\mathrm{m}^2$	permeability host medium
k_l	$5.3 \times 10^{-12}\,\mathrm{m}^2$	permeability lens
p_e^h	2218 Pa	entry pressure host medium
p_e^l	2550 Pa	entry pressure lens
$2d$	0.04 m	width of opening
$2L$	1.12 m	length of lens
H	0.10 m	depth of lens
λ	2.48	parameter Brooks–Corey model
μ_w	$1.00 \times 10^{-3}\,\mathrm{Pa\,s}$	viscosity water
μ_n	$0.57 \times 10^{-3}\,\mathrm{Pa\,s}$	viscosity DNAPL
ρ_w	$1.00 \times 10^{+3}\,\mathrm{kg\,m^{-3}}$	density water
ρ_n	$1.46 \times 10^{+3}\,\mathrm{kg\,m^{-3}}$	density DNAPL

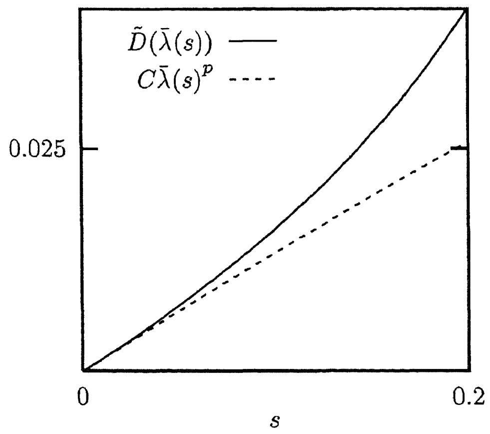

Figure 5. Small saturation approximation for Brooks–Corey function with $\lambda = 2.48$.

For the numerical calculation we use a finite computational domain $\Omega = (0, 0.2) \times (0, 0.4)$. Here we have taken advantage of the symmetry of the problem. At the boundaries of this computational domain we impose $n \cdot q_t = 0$, except at $x = 0.2$, and

$$\begin{cases} n \cdot q_n = 0, & z = 0,\ x > d, \\ n \cdot q_n = -q_n^i, & z = 0,\ x \leqslant d, \\ n \cdot \mathrm{grad}\, s = 0, & z = 0.4, \\ s = 0,\ p = \rho_w g z, & x = 0.2. \end{cases} \tag{64}$$

These boundary conditions imply a hydrostatic pressure distribution at the side boundaries, and negligible capillary diffusion at the bottom of the computational domain.

The problem is discretized on a grid with a mesh size of 0.0025 m in both coordinate directions. The steady-state solution is obtained by putting the porosity

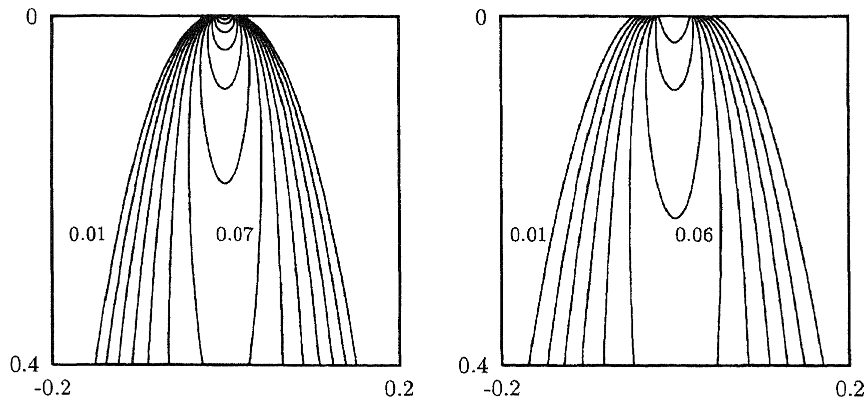

Figure 6. Barenblatt–Pattle solution (left) and numerical solution (right). Contour levels are at equidistant intervals of 0.01, the outermost contour representing a nonwetting phase saturation of 0.01.

ϕ equal to 0 in equations (55)–(56). The fine grid solution is obtained by a nested iteration procedure. First the solution is calculated on a coarse grid, and this solution is then interpolated to a next finer grid. On all grids we use the multigrid procedure to solve the discrete equations.

In figure 6 contour plots of the DNAPL saturation are shown for the explicit solution (34) and the numerical solution. We observe that the solutions differ slightly directly underneath the opening. This is expected, because the explicit solution is obtained for a different boundary condition in the opening. However, the approximation of the plume width as well as the qualitative agreement between the two solutions is very good.

Note that ignoring the capillary forces in the vertical direction leads, in view of (17), to an over- or underprediction of the density induced flux, or equivalently of the DNAPL saturation, depending on the sign of the capillary pressure gradient in downward direction for the unapproximated problem. This is consistent with the observation that at points where the saturation gradient for the numerical solution in figure 6 is negative in the downward direction, the saturation for the analytical approximation is slightly overpredicted, whereas at points where it is positive, the saturation is slightly underpredicted.

We remark that the full unapproximated steady-state flow problem is completely determined by the dimensionless numbers N_{cg}, N_q, M, given in (22), and the ratio $\Delta\rho/\rho_w$. Higher values of the absolute permeability while keeping other parameters unchanged yield smaller N_{cg} and N_q in view of (14) and (22). From (19), (36) and figure 5 we observe that the quality of the approximations improves for smaller values of N_{cg} or N_q. Thus higher values of the permeability lead to an improvement of the quality of the explicit solution shown here. This conclusion is still valid when the specific discharge in the opening is chosen proportionally higher, so that N_q remains unchanged and only N_{cg} is smaller.

4.2.2. DNAPL infiltration into low-permeable lens

Let us now verify criterion (49) for DNAPL infiltration into a lens with higher entry pressure than the surrounding host medium. For the data given in table 1 we have the critical saturation $s^* \approx 0.29$, and the critical DNAPL discharge $Q_i^* \approx 2.64 \times 10^{-9}$ m^{2}s^{-1} for steady infiltration. We consider transient DNAPL infiltration for $Q_i = 1.24 \times 10^{-9}$ m^{2}s^{-1} and $Q_i = 5.40 \times 10^{-9}$ m^{2}s^{-1}, so approximately half and twice the critical discharge Q_i^*, respectively.

Before we proceed to the computational results, we first check whether the DNAPL plume in the case without lens has small width compared with the lens. Using the Barenblatt–Pattle solution, it follows from equation (35) that the full width of the DNAPL plume is given by $2d(1 + 331.7z)^{0.43}$, so for $H = 0.1$ m the ratio of the unperturbed DNAPL plume width and the length of the lens is 0.16. For the simulations we use as computational domain $\Omega = (0, 0.8) \times (0, 0.28)$. The boundary conditions are, apart from the location of bottom and side boundaries, equal to (64). The mesh width in our computations is 0.005 m, which implies a 160×56 grid.

First we consider the case of slow infiltration ($Q_i = 1.24 \times 10^{-9}$ m^{2}s^{-1}). Contour plots of the numerical solution are shown in the left hand column of figure 7. The solution is shown after approximately 125, 375 and 750 hours. When the DNAPL plume reaches the lens, the DNAPL saturation is too low to overcome the entry pressure ($s^* \approx 0.29$). It spreads laterally in response to capillary pressure gradients, and reaching the end of the lens, it drops off. DNAPL does not penetrate the lens in accordance with criterion (49) for steady DNAPL infiltration. We remark that the assumption $s \approx 0$ at the end of the lens is indeed borne out in practice.

Next we consider the case of fast DNAPL infiltration ($Q_i = 5.40 \times 10^{-9}$ m^{2}s^{-1}). In the right hand column of figure 7 contour plots of the solution are shown after approximately 25, 125 and 250 hours. As in the previous case, the DNAPL plume first spreads laterally after reaching the lens. However, in this case the lateral transport of DNAPL due to capillary forces is too slow compared to the supply of DNAPL. Right underneath the opening the DNAPL saturation is largest. There it exceeds the critical saturation s^* and DNAPL starts to infiltrate into the lens. After 250 hours a substantial part of the lens has been penetrated by DNAPL.

We observe that the agreement between the analytical and numerical results with regard to the qualitative flow behavior is very good. The Barenblatt–Pattle solution provides a useful estimation of the width of the downward migrating DNAPL plume. Note that this plume is narrower for the slow infiltration case. Moreover, criterion (49) derived for steady-state infiltration appears to hold for the practically relevant case of transient infiltration.

As in the homogeneous case, the quality of the approximations will improve for higher values of the permeability. The approximation of the downward migrating plume will be better as well as the quality of the Vertical Equilibrium assumption above the lens due to improved vertical communication. Note that the critical discharge Q_i^* defined in (49) is invariant for different values of the host permeability in view of (14) provided that the entry pressure ratio (and thus s^*) is not changed.

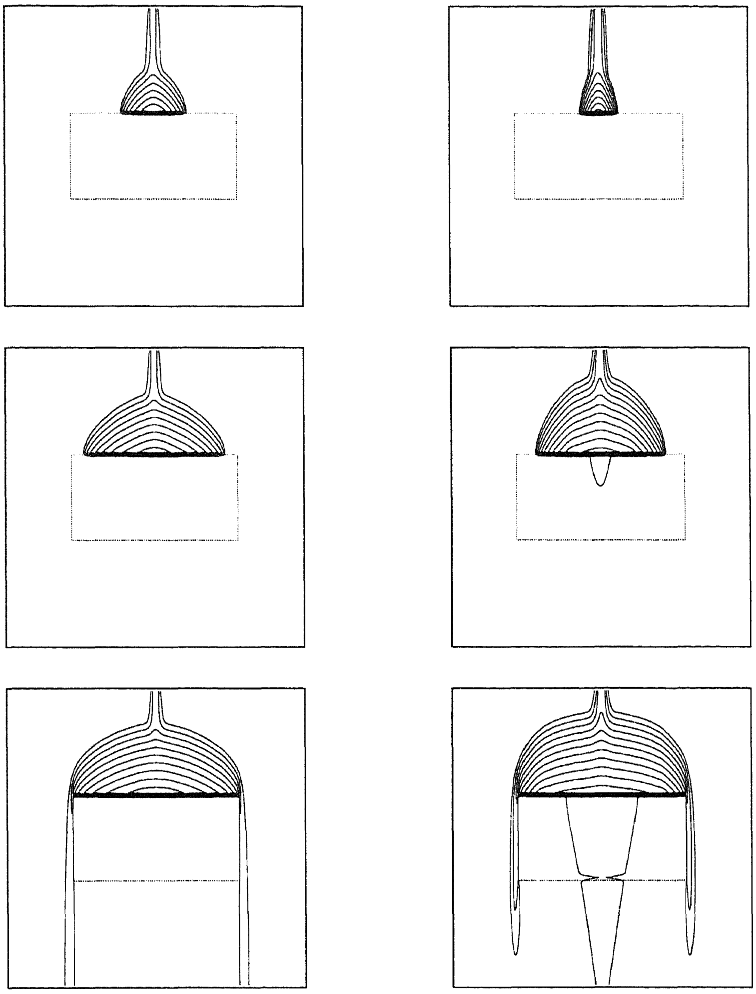

Figure 7. Numerical results for the problem with a single lens. Contour levels are at equidistant intervals of 0.025, the outermost contour representing a nonwetting phase saturation of 0.025. Left: slow infiltration ($Q_\mathrm{i} = 1.24 \times 10^{-9}$ m^{2}s^{-1}) at $T = 125$, 375 and 750 hr. Right: fast infiltration ($Q_\mathrm{i} = 5.40 \times 10^{-9}$ m^{2}s^{-1}) at 25, 125 and 250 hr.

We remark that in the numerical example we have chosen a relatively small difference between the entry pressures. The threshold saturation s^* is then sufficiently low, so that also in the case of penetration of the lens the total flow can be disregarded in view of (50). Recall that the criterion for DNAPL penetration (49) has been derived under the assumption of zero total flow. The value of Q_i^* may therefore not be correct for greater entry pressure ratios and correspondingly higher threshold saturations s^*. However, for sufficiently small $\widetilde{s}$ satisfying (50), we have from (47) that the saturation on the lens boundary must be less than $\widetilde{s}$ if $Q_\mathrm{i} \leqslant \widetilde{Q}_\mathrm{i}$, where $\widetilde{Q}_\mathrm{i}$ follows from (49) with

s^* replaced by $\widetilde{s}$. Thus we may conclude that also for higher entry pressure contrasts DNAPL does not penetrate the lens if the discharge in the opening is sufficiently low.

5. Conclusion

We have studied the problem of DNAPL infiltration. For the homogeneous case we derived an upper bound of the DNAPL plume width as well as an explicit solution governing the DNAPL plume for small saturations. For the problem with a single lens we derived an explicit expression for the critical DNAPL inflow. If this critical discharge is exceeded DNAPL infiltrates into the lens.

Several numerical simulations were carried out. The simulations show a good agreement between the analytical and numerical results with regard to the qualitative flow behavior. In the homogeneous case, the explicit solution indeed gives a good estimate of the DNAPL plume width. Moreover, the criterion for the critical DNAPL discharge appears to be valid for the practically relevant case of transient infiltration.

References

[1] F.V. Atkinson and L.A. Peletier, Similarity profiles of flows through porous media, Arch. Rat. Mech. Anal. 42 (1971) 369–379.

[2] R.H. Brooks and A.T. Corey, Hydraulic properties of porous media, Colorado State University (1964).

[3] G. Chavent and J. Jaffre, *Mathematical Models and Finite Elements for Reservoir Simulation*, Studies in Mathematics and Applications 17 (Elsevier, Amsterdam, 1986).

[4] G. Chavent, J. Jaffre and J.E. Roberts, Mixed-hybrid finite elements and cell-centered finite volumes for two-phase flow in porous media, in: *Mathematical Modelling of Flow through Porous Media*, eds. A.P. Bourget, C. Carasso, S. Luckhaus and A. Mikelic (World Scientific, 1995) pp. 100–114.

[5] M.I.J. van Dijke, S.E.A.T.M. van der Zee and C.J. van Duijn, Multi-phase flow modeling of air sparging, Adv. Water Resources 18(6) (1995) 319–333.

[6] C.J. van Duijn, J. Molenaar and M.J. de Neef, Effects of capillary forces on immiscible two-phase flow in heterogeneous porous media, Transport in Porous Media 21 (1995) 71–93.

[7] C.J. van Duijn and L.A. Peletier, A class of similarity solutions of the nonlinear diffusion equation, Nonlinear Analysis, Theory, Methods and Applications 1 (1977) 223–233.

[8] A. Friedmann and S. Kamin, The asymptotic behaviour of a gas in an n-dimensional porous medium, Trans. Amer. Math. Soc. 262 (1980) 551–563.

[9] M.Th. Van Genuchten, A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Sciences Society of America Journal 44 (1980) 892–898.

[10] R. Helmig, M. Emmert and H. Sheta, Modelling of multiphase flow in heterogeneous porous media and applications, in: *Proc. of the 6th Int. Conf. on Computing in Civil and Building Engineering* (1995).

[11] B.H. Kueper, W. Abbott and G. Farquhar, Experimental observations of multiphase flow in heterogeneous porous media, J. Contam. Hydrol. 5 (1989) 83–95.

[12] B.H. Kueper and E.O. Frind, Two-phase flow in heterogeneous porous media – 1. Model development, Water Resour. Res. 27 (1991) 1049–1057.

[13] B.H. Kueper and E.O. Frind, Two-phase flow in heterogeneous porous media – 2. Model application, Water Resour. Res. 27 (1991) 1059–1070.

[14] M.C. Leverett, Capillary behavior in porous solids, Trans. AIME, Petr. Eng. Div. 142 (1941) 152–169.

[15] J. Molenaar, Multigrid methods for fully implicit oil reservoir simulation, Technical Report, T.U. Delft (1995). To appear in *Proceedings Copper Mountain Conference on Multigrid Methods*, 1995.

[16] O.A. Oleinik, S.N. Kalashnikov and Y.L. Chzhou, The Cauchy problem and boundary problems for equations of the type of nonstationary filtration, Izv. Akad. Nauk. SSSR Ser. Mat. 22 (1958) 667–704.

[17] D.W. Peaceman, *Fundamentals of Numerical Reservoir Engineering* (Elsevier, 1977).

[18] L.A. Peletier, The porous medium equation, in: *Applications of Nonlinear Analysis in the Physical Sciences*, eds. H. Amann, N. Bazley and K. Kirchgässner (Pitman, 1981) pp. 229–241.

[19] M.H. Protter and H.F. Weinberger, *Maximum Principles in Differential Equations* (Prentice-Hall, Englewood Cliffs, NJ, 1967).

[20] J.L. Vázquez, An introduction to the mathematical theory of the porous medium equation, in: *Shape Optimization and Free Boundaries*, eds. M.C. Delfour and G. Sabidussi (Kluwer, Dordrecht, 1992) pp. 347–389.