Cornelis Johannes van Duijn
Executive Board
Eindhoven University of Technology
c.j.v.duijn@tue.nl

Iuliu Sorin Pop
Mathematics and Computer Science
Eindhoven University of Technology
i.pop@tue.nl

Shock waves and two phase porous media flows

Models for porous media flow with multiple fluids (water and oil, for example) are important for studying techniques such as geological storage of CO_2 and water driven oil recovery. These models consist of conservation laws and often contain nonlinearities that preclude the existence of classical solutions. Hans van Duijn and Sorin Pop discuss important aspects of the theory of hyperbolic conservation laws, in particular existence and uniqueness of weak solutions, admissibility conditions and shock solutions. This theory explains saturation overshoots occurring in porous media flows under non-equilibrium conditions.

Mathematical models and simulation tools are essential for an optimal exploitation of geological resources. In many cases, for instance groundwater flow, water driven oil recovery, or geological CO_2 storage [1, 7, 12], the underlying mathematical models consist of conservation laws. These are nonlinear evolution equations having either a hyperbolic or a parabolic character. The nonlinearities and data appearing in the models allow for the existence of so-called weak solutions, i.e. discontinuous solutions. The weak solutions are defined, based on test functions and partial integration. Natural questions arising in this context are existence, uniqueness, and regularity of these solutions. For parabolic problems, uniqueness generally holds. This is not the case of hyperbolic problems, where uniqueness requires additional admissibility conditions, leading to so-called *entropy solutions*.

In this paper we discuss two admissibility concepts. They are based on the observation that hyperbolic equations arise from evolution equations involving higher order derivatives, by letting such terms vanish. In porous media models, this is similar to vanishing capillarity.

Flows in porous media

In this paper we analyze a model that describes the flow of two incompressible and immiscible fluids through a porous medium. Such models arise in geological CO_2 storage. We follow the approach in which the porous medium is considered as a continuum, characterized by averaged properties such as porosity ϕ and permeability K. The presence of each fluid is described by a saturation, S_w for water and S_n for CO_2. The model equations arise from a combination of mass balance and Darcy laws for both fluids [1, 7]. When restricting ourselves to horizontal flows through homogeneous reservoirs, the following one-dimensional description results (with $\alpha \in \{w, n\}$):

$$\phi \frac{\partial S_\alpha}{\partial t} + \frac{\partial v_\alpha}{\partial x} = 0 \quad \text{(mass balance)}, \tag{1}$$

$$v_\alpha = -K \frac{k_{r\alpha}}{\mu_\alpha} \frac{\partial p_\alpha}{\partial x} \quad \text{(Darcy)}. \tag{2}$$

For each fluid, v_α is the averaged velocity, μ_α the dynamic viscosity and p_α the pressure in fluid α. Furthermore, $k_{r\alpha}$ denotes the relative permeability of fluid α. Experiments show that it is an increasing function of the corresponding fluid saturation, i.e.

$$k_{r\alpha} = k_{r\alpha}(S_\alpha). \tag{3}$$

One can insert (2) into (1) to reduce the system to two equations, involving, however, four unknowns, two saturations and two pressures. To close the system one assumes the pores are occupied completely by the two fluids (thus no other fluid or void is present), implying

$$S_w + S_n = 1. \tag{4}$$

The difference of the fluid pressures, called *capillary pressure*, depends on the CO_2 saturation S_n. In standard models it is given by

$$p_n - p_w = P_c(S_n), \tag{5}$$

where P_c is strictly increasing.

From (1) and (4) one concludes that the sum of the fluid velocities, $v = v_n + v_w$, is constant in space. It remains constant in time too if the injection process is at constant flow rate. Introducing reference quantities the model reduces to one scalar equation

$$\partial_t u + \partial_x f(u) = \varepsilon\Big(H(u)\partial_x P\Big) \quad \text{for all } t > 0 \text{ and } x \in \Omega, \tag{6}$$

which involves only one dimensionless number ε, the *capillary number*. This is related to the ratio of viscous forces and surface tension acting across the interface between the two fluids.

In (6) u denotes the CO_2 saturation, $u = S_{\mathrm{n}}$, P is the dimensionless capillary pressure and Ω is the dimensionless interval of interest. Below we consider $\Omega = \mathbb{R}$. The nonlinear functions are:

$$\begin{aligned} f(u) &= \frac{k_o(u)}{k_o(u) + M k_w(u)}, \\ H(u) &= k_w(u) f(u). \end{aligned} \tag{7}$$

Typically, the function f has a convex-concave profile.

In view of (5) one has

$$P = P(u). \tag{8}$$

Common choices in the porous media literature are

$$\begin{aligned} &k_o(u) = u^{1+p}, \quad k_w(u) = (1-u)^{1+q} \\ &\text{and } P(u) = (1-u)^{-\frac{1}{\lambda}}, \end{aligned}$$

where $p, q > 0$, $\lambda > 1$ and $M > 0$ are model specific, [1].

Non-equilibrium models

The above-mentioned model is based on permeability — saturation and capillary pressure — saturation functions under so-called 'equilibrium conditions'. In this case, measurements are performed after achieving a static distribution of the fluids inside the pores. However, capillary pressure functions measured under non-equilibrium conditions, when the fluids do not reach a steady state, are different from those under equilibrium ones. Further, unexpected saturation profiles have been measured in [2] for infiltration in a thin and long column filled by homogeneous sand. As shown in Figure 1, the saturation profiles for a low flux at the inflow are monotone, as predicted by equilibrium models (see e.g. [10]). For higher fluxes, so-called 'saturation overshoots' are observed: at the infiltration front, the saturation values are higher than the ones at the influx. As the flux increases, this profile becomes even more intriguing: a saturation plateau that is higher than the inflow saturation appears between an infiltration front and a drainage front.

Such non-monotonic saturation profiles are ruled out by equilibrium models, therefore non-equilibrium ones are required. A model incorporating dynamic effects in the capillary pressure is proposed in [6], where (5) becomes

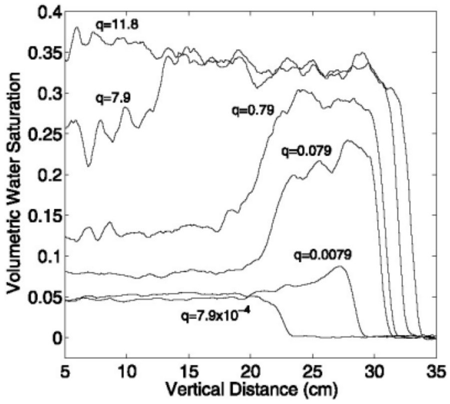

Figure 1 Saturation profiles measured for different fluxes (courtesy of D.A. DiCarlo); note that these profiles become non-monotonical with the increase of the flux.

$$P_{\mathrm{c}} = P^e_{\mathrm{c}}(S_{\mathrm{n}}) + \hat{\tau}\, \partial_t S_{\mathrm{n}}. \tag{9}$$

P^e_{c} is the capillary pressure-saturation function determined under equilibrium. The second term accounts for the non-equilibrium effects. The parameter $\hat{\tau}$ is assumed constant for simplicity; generally it may depend on S_{n}. In the simplified, dimensionless setting considered here, the capillary pressure becomes

$$P = P(u) + \varepsilon\tau\partial_t u, \tag{10}$$

with the dimensionless *dynamic number* τ. Then (6) reads

$$\begin{aligned} &\partial_t u + \partial_x f(u) \\ &\quad = \varepsilon\Big(H(u)\partial_x(P(u) + \tau\varepsilon\partial_t u)\Big), \end{aligned} \tag{11}$$

for all $t > 0$ and $x \in \mathbb{R}$.

Remark. Both dimensionless numbers ε and τ depend on the reference quantities, see [11]. In particular, the dynamic number is proportional to the square of the reference velocity. In other words, a higher flux at the inflow results in a higher value for τ. This is a key observation for explaining the occurrence of saturation overshoots.

Admissible shocks

Formally, when letting ε tend to 0, both (6) or (11) become:

$$\partial_t u + \partial_x f(u) = 0 \quad \text{for } t > 0, x \in \mathbb{R}. \tag{12}$$

This equation is hyperbolic. We consider *Riemann* initial data,

$$u(0,x) = u_0(x) = \begin{cases} u_\ell & \text{if } x < 0, \\ u_r & \text{if } x > 0, \end{cases} \tag{13}$$

with given states $u_\ell, u_r \in \mathbb{R}$. We only consider bounded solutions, satisfying

$$\begin{aligned} &\lim_{x\to-\infty} u(t,x) = u_\ell \\ \text{and} \quad &\lim_{x\to\infty} u(t,x) = u_r \end{aligned} \tag{14}$$

for all $t > 0$. Moreover, since u is the CO_2 saturation, we only consider states satisfying $0 \le u_\ell, u_r \le 1$.

Having formulated the initial value problem (12)–(13), a natural question arising is the existence and uniqueness of solutions. Without entering into details, we mention that *classical solutions* fail to exist. Alternatively, one can multiply the original equation by a *test function* φ and integrate the resulting equation over the time-space domain. After integration by parts, a *weak solution* is defined as a bounded, measurable function satisfying

$$\begin{aligned} &\int_0^\infty \int_{\mathbb{R}} u\partial_t\varphi + f(u)\partial_x\varphi \, dx\, dt \\ &\qquad + \int_{\mathbb{R}} u_0(x)\varphi(0,x)\, dx = 0, \end{aligned} \tag{15}$$

for all $\varphi \in C^1_0([0,\infty)\times\mathbb{R})$, the space of continuously differentiable functions that vanish uniformly for large t and x. Clearly, any classical solution is also a weak solution, but the latter class is much wider. In particular, a weak solution may even be discontinuous.

The existence of a solution can be proved in the context above. However, uniqueness remains an open question, as this does not hold generally. For example, consider the *Burgers* equation,

$$\partial_t u + \partial_x\Big(\frac{1}{2}u^2\Big) = 0 \quad \text{for } t > 0,\ x \in \mathbb{R}. \tag{16}$$

Let the initial condition in (13) with $u_\ell = 0$ and $u_r = 1$. One can verify that both functions given below are weak solutions:

$$u_a(t,x) = \begin{cases} 0 & \text{if } x \le 0, \\ \dfrac{x}{t} & \text{if } 0 < x < t, \\ 1 & \text{if } x \ge t, \end{cases}$$

$$u_b(t,x) = \begin{cases} 0 & \text{if } x < \dfrac{1}{2}t, \\ 1 & \text{if } x > \dfrac{1}{2}t. \end{cases}$$

Note that u_a is a continuous transition from the left state $u_\ell = 0$ to the right state $u_r = 1$. These states are connected by a fan that becomes wider in time; such solutions are called *rarefaction waves*. At the same time, u_b is a *shock*, a jump from u_ℓ to u_r. This shock is located at $x(t) = \frac{1}{2}t$ and travels with a fixed velocity $s = x'(t) = \frac{1}{2}$. The shock satisfies the general *Rankine–Hugoniot* condition relating the shock speed to the states at its left and right sides,

$$s = \frac{f(u_\ell) - f(u_r)}{u_\ell - u_r}, \tag{17}$$

where f is the *flux function* in the conservation law (12). In general, one can prove that functions having discontinuities travelling with a velocity that respects (17), and satisfying the equation in classical sense away from the shock, are weak solutions (see e.g. [5]). This rises another question: *which solution is relevant?* In other words, additional criteria are required for selecting the weak solution of interest.

A natural approach is to use underlying physics and to investigate which structure has been lost by letting ε tend to zero in the original, *regularized* model. In particular, since the shock profiles are constant in time, one can think of similar solutions to the regularized model, *travelling waves* (TW). Such waves connect the same left and right states as the shock. In other words, one investigates solutions u^ε to the regularized equation, having the structure

$$u^\varepsilon(t,x) = v(\eta), \quad \text{with } \eta = (x - st)/\varepsilon, \tag{18}$$

and satisfying

$$\lim_{\eta\to-\infty} v^\varepsilon(\eta) = u_\ell \quad \text{and} \quad \lim_{\eta\to\infty} v^\varepsilon(\eta) = u_r. \tag{19}$$

A shock u is called *admissible* if it is the limit of a TW solution:

$$u(t,x) = \lim_{\varepsilon\to 0} v^\varepsilon(x - st). \tag{20}$$

Note that neither (6) nor (11) depend explicitly on t or x, so any translation of a TW remains a TW. Therefore we fix the wave by assuming that $v^\varepsilon(0) = (u_\ell + u_r)/2$.

In what follows we concentrate on shock solutions to (12), satisfying (in the sense of left and right limits)

$$\lim_{x\nearrow st} u(t,x) = u_\ell \quad \text{and} \quad \lim_{x\searrow st} u(t,x) = u_r. \tag{21}$$

Such shocks will be denoted by $\{u_\ell, u_r\}$. Following the above, we call the shock $\{u_\ell, u_r\}$ admissible if it is the limit ($\varepsilon \to 0$) of a TW v^ε connecting u_ℓ to u_r.

Oleinik's criterion

In the classical theory for hyperbolic conservation laws, a generally accepted admissibility criterion is due to O.A. Oleinik (see [9], Chapter II) and is based on the parabolic regularization of (12). In the context of two-phase flow in porous media, we consider (6) with the capillary pressure in (8). This deviates slightly for the standard approach, where the terms on the right are replaced by $\varepsilon\partial_{xx}u$. We seek TW solutions u^ε to (6), satisfying (21), and having the structure stated in (18). We assume that the waves v are smooth, i.e., twice continuously differentiable. Applying the chain rule, and integrating the resulting once with respect to η leads to

$$\begin{cases} A - sv + f(v) = H(v)\big(P(v)\big)' \text{ for } \eta \in \mathbb{R}, \\ \lim_{\eta\to-\infty} v(\eta) = u_\ell \text{ and } \lim_{\eta\to\infty} v(\eta) = u_r, \end{cases} \tag{22}$$

with $A, s \in \mathbb{R}$ to be determined. Note that the scaling in (18) allows eliminating ε from (22). However, if a TW solution exists, the profile of the corresponding u^ε becomes steeper as ε tends to 0. In the limit, this leads to a shock solution to (12).

The behaviour of v as $\eta \to \pm\infty$ implies that the term on the right in (22) tends to 0 as well, yielding

$$s = \frac{f(u_\ell) - f(u_r)}{u_\ell - u_r} \quad \text{and } A = \frac{u_r f(u_\ell) - u_\ell f(u_r)}{u_\ell - u_r}. \tag{23}$$

Note that the TW speed is the shock speed introduced in (17). With $\beta(v) = \int H(v)P'(v)dv$, a solution of (22) solves

$$\big(\beta(v)\big)' = g(v) := A - sv + f(v), \quad \text{for } \eta \in \mathbb{R}, \tag{24}$$

subject to the initial condition $v(0) = (u_\ell + u_r)/2$.

Clearly, (23) is necessary, but not sufficient for the existence of TW solutions, as the latter implies that the solution of (24) also has the asymptotic behaviour (22). This behaviour can be reinterpreted in terms of phase plane analysis, where u_ℓ acts as a source-type equilibrium, and u_r as a sink. Moreover, (24) should have no equilibria between the two states u_ℓ and u_r. This means that the term on the right in (24) does not vanish between the two states, hence g has a constant sign there. This shows that the waves are monotone. In mathematical terms, this becomes the celebrated *Oleinik entropy condition*, saying that shocks $\{u_\ell, u_r\}$ are admissible if and only if for all v between u_ℓ and u_r,

$$\frac{f(v) - f(u_\ell)}{v - u_\ell} \geq s \geq \frac{f(v) - f(u_r)}{v - u_r}. \tag{25}$$

In particular, for (16) this implies that shocks $\{u_\ell, u_r\}$ are admissible if and only if $u_\ell > u_r$. Hence u_b is not admissible in the sense of Oleinik.

For model (6), where f has a convex-concave profile, this means that, if $u_\ell > u_r$, shocks $\{u_\ell, u_r\}$ are admissible only if the segment connecting the points $(u_\ell, f(u_\ell))$ and $(u_r, f(u_r))$ is above the graph of f and has no interior intersection points with the graph. For example, a shock $\{1, 0\}$ is not admissible in this case. A general feature of admissible shocks (according to this criterion) is that characteristics from the left and right sides of a shock converge into the shock (as time is increasing).

Non-classical shocks

Oleinik's approach uses a parabolic regularization of the hyperbolic equation (12), which corresponds to the equilibrium capillary pressure model (5). The TW solutions discussed before remain monotone. As mentioned, there are experimental results contradicting this monotonicity, which justifies non-equilibrium models as (11).

In this respect, one question is whether such models can justify *non-classical* shock solutions to (12), which violate Oleinik's admissibility condition (25). We refer to [9], where 'connectable' left and right states, or admissible shocks $\{u_\ell, u_r\}$, are defined based on a predefined *kinetic function*. Similarly, in [4] admissible shocks $\{u_\ell, u_r\}$ are defined as the limit $\varepsilon \to 0$ of TW solutions to (11), and satisfying (22).

From a physical point of view, such shocks are obtained in the vanishing capillary pressure limit of two-phase porous media flow models, when dynamic effects are included in the capillary pressure. Clearly, such shocks depend on τ; for $\tau = 0$ one obtains the classical shocks in the previous subsection. Although formally the limit equation (12) rem-

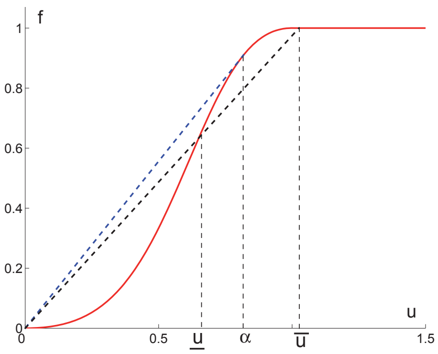

Figure 2 The function f for $p = 1$, $q = 1$ and $M = 2$; here α is the tangent point.

ains the same for any τ, the case $\tau > 0$ leads to important differences in the structure of the TW solutions and consequently in the admissibility of shocks. With (22), we seek v solving

$$\begin{cases} H(v)\big(s\tau v' - P(v)\big)' = A - sv + f(v), & \\ \qquad\qquad \text{for } \eta \in \mathbb{R}, & (26) \\ \lim\limits_{\eta\to-\infty} v(\eta) = u_\ell \text{ and } \lim\limits_{\eta\to\infty} v(\eta) = u_r, & \end{cases}$$

with s given by (23). Moreover, A has the same value, at least if H does not vanish; the *degenerate* case, when $H(u) = 0$ for e.g. $u = 0$ and $u = 1$, is analyzed in [3].

The existence of TW depends on τ. Here we consider $u_r < u_\ell$, and let α be the point where the tangent line through $(u_r, f(u_r))$ touches the graph of f (see Figure 2). In this context, the following results are proved in [4]:

Theorem. *If $u_r < \alpha \le u_\ell$, there exists $\tau_* > 0$ such that:*

a. If $0 \le \tau \le \tau_*$, TW connecting $u_\ell \le \alpha$ to u_r exist and are monotone.

b. If $\tau > \tau_*$, there exists a unique $\bar{u}_\ell(\tau) > \alpha$ that can be connected to u_r through a monotone TW.

c. The $\bar{u} - \tau$ dependency is continuous and increasing for $\tau \ge \tau_*$.

If $\tau > \tau_*$, with $u_\ell = \overline{u}(\tau)$, let $\underline{u}(\tau) \in (u_r, \alpha)$ be the u-coordinate of the middle intersection point of the graph of f with the chord through $(u_\ell, f(u_\ell))$ and $(u_r, f(u_r))$. Then

d. For each $u_\ell \in (u_r, \underline{u}(\tau)]$, there exists a TW connecting u_ℓ to u_r.

e. For each $u_\ell \in (\underline{u}(\tau), \bar{u}(\tau))$, no TW connecting u_ℓ to u_r exist.

f. For each $u_\ell \in (\underline{u}(\tau), \bar{u}(\tau))$, TW connecting u_ℓ to $\bar{u}(\tau)$ are possible.

Given u_r, Figure 3 displays the values $\bar{u}(\tau)$ and $\underline{u}(\tau)$ for different values of τ. These points are computed by a shooting method (see [3]).

Case b of the theorem provides TW solutions connecting $u_\ell = \bar{u}(\tau) > \alpha$ to u_r. Letting $\varepsilon \to 0$, this TW justifies a shock solution $\{u_\ell, u_r\}$ to (12) that violates (25), which states that shocks $\{u_\ell, u_r\}$ are admissible only if $u_\ell \in (u_r, \alpha]$. If the choice of u_r, u_ℓ and τ places us the case f, the solution of the Riemann problem (12)–(13) combines two shocks: one upwards $\{u_\ell, \bar{u}(\tau)\}$ and one downwards $\{\bar{u}(\tau), u_r\}$. This is again a non-classical construction, where the solution is a shock down to u_r, possibly preceded by a rarefaction wave from u_ℓ to α if $u_\ell > \alpha$. This behaviour is displayed in Figure 4, presenting two numerical solutions computed for the regularized models with $\tau > \tau_*$, respectively $\tau = 0$. The former presents two fronts corresponding to the shocks mentioned before, the latter only one front connecting α to $u_r = 0$.

Saturation overshoot

The travelling wave analysis in the previous section provides the mathematical framework for explaining the occurrence of non-monotonic saturation profiles during infiltration. As observed in Figure 1, at low fluxes the saturation has a monotone profile. In this case, dynamic effects are negligible. The situation is changing as the flux is increasing; as mentioned before in a remark, a higher flux translates into a higher value of the parameter τ in the dimensionless setting. To relate the TW construction with the experiments, we mention that the left state u_ℓ represents the saturation at the inflow, whereas the right state u_r is nothing but the initial saturation (clearly, satisfying $u_r < u_\ell$). Then, as follows from the theorem, whenever

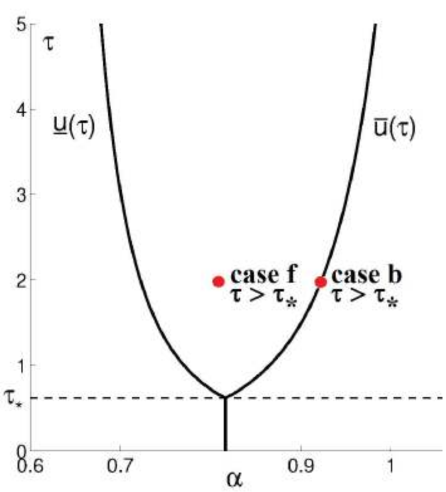

Figure 3 The branches $\bar{u}(\tau)$ (right) and $\underline{u}(\tau)$ (left) computed for $u_r = 0$. With $\tau > \tau_*$, in case b of the theorem $u_\ell = \bar{u}(\tau)$, while in case f $u_\ell \in (\underline{u}(\tau), \bar{u}(\tau))$.

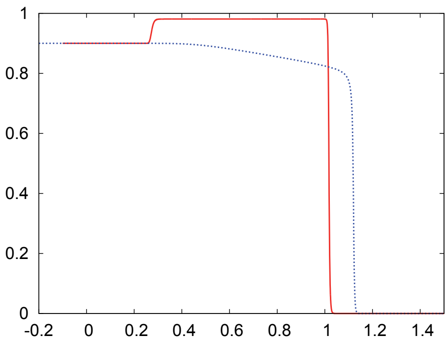

Figure 4 Numerical solutions for the full model (12), $\tau > \tau_*$ (solid) and $\tau = 0$ (dotted).

$\tau < \tau_*$, if $u_\ell < \alpha$, TW connecting u_ℓ to u_r are possible, also providing a monotonic saturation profile.

Increasing the flux at inflow has two implications in the dimensionless model: an increase of τ, as well as of u_ℓ. In this case, the theorem rules out the possibility of TW connecting u_ℓ directly to u_r. Instead, two fronts are encountered: an infiltration front from $\bar{u}(\tau)$ down to u_r and a drainage front from $\bar{u}(\tau)$ to u_ℓ. Between the two fronts, the saturation has a constant, *plateau* value $\bar{u}(\tau)$. These are also the saturation profiles in Figure 1, determined experimentally at high fluxes.

The present discussion is restricted to homogeneous media in one spatial dimension. Of course, realistic situations require two- or three-dimensional models, and heterogeneous media. One interesting phenomenon in the multi-dimensional case appears during infiltration in homogeneous media, when preferential flow is encountered in some parts of the medium. This leads to the development of *fingers*, which are thin regions of high saturation embedded into regions of low saturation. Such profiles are again ruled out by standard, equilibrium models, but permitted in the non-equilibrium case. Figure 5 presents such profiles, computed for the model (12) by a heterogeneous multiscale scheme (see [8]).

From practical point of view, the occurrence of preferential flow paths impacts the performance of the system. For example, in water driven oil recovery, when injecting water to displace oil, a water saturation overshoot implies that less oil is left in the reservoir. However, as seen above such overshoots are associated with the formation of fingers: inside fingers a high water saturation is encountered, whereas outside the saturation remains low. Water will prefer flowing through the fingers, leaving much oil unmobilized outside fingers. This reduces significantly the oil production. Similarly, when injecting supercritical CO_2 in the sub-surface, having fingers

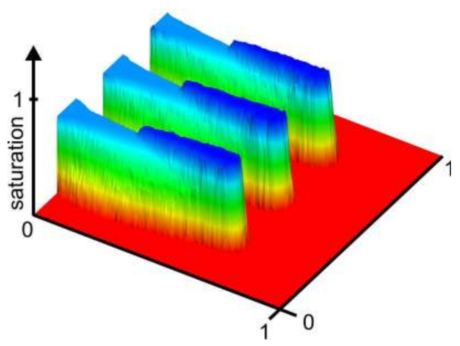

Figure 5 Fingers developed during infiltration in a heterogeneous medium (courtesy of F. Kissling). Note that even along a finger the saturation profile is non-monotone.

and preferential flow paths means that much of the storage reservoir is not reached by the CO_2 and therefore left unused. A proper management of such systems is based on the thorough understanding of the processes at various scales. This includes taking into account dynamic effects in controlling the flow regimes, so that the global efficiency is not depleted.

Conclusion

We discussed two mathematical models for two-phase flows in porous media. The difference between the two models is in the capillary pressure-saturation dependency. In standard (equilibrium) models this is a nonlinear, monotone function, whereas non-equilibrium models also include the time derivative of the saturation. In both approaches, we let the capillary effects tend to zero to obtain admissibility conditions for shock solutions of the limit hyperbolic equation. These conditions depend on the parameter τ appearing in the dynamic capillarity term. We also discuss how non-equilibrium models can explain the saturation overshoot in the infiltration profiles, which are measured experimentally, but ruled out by the equilibrium theory.

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