# CO<sub>2</sub> VERTICAL MIGRATION THROUGH A LAYERED POROUS MEDIUM : DYNAMICS AND UPSCALING

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**Summary.** We analyze the vertical migration of a  $CO_2$  plume through a periodic layered porous medium made up of high and low permeability layers and initially filled with water. The two-phase flow model is based on the Buckley-Leverett equation including gravity effects. In a first step we show how the flux continuity at the interfaces leads to saturation discontinuities and correlatively to  $CO_2$  stratification as modelled in 2D or 3D aquifers. Then the impact of relative permeabilities discontinuity between layers is discussed and the correlation between the wettability of the layers and the  $CO_2$  saturation spatial distribution is investigated. Finally we propose an upscaled transport model based on homogeneization in periodic structures and we compare the upscaled solution with the exact numerical solution.

## **1 INTRODUCTION**

Potential geological storage sites for the sequestration of carbon dioxide (CO<sub>2</sub>), like deep saline aquifers or gas and oil reservoirs, are heterogeneous. According to Ambrose et al.<sup>1</sup> two types of heterogeneity can be considered : stratigraphic heterogeneity and structural heterogeneity (faults or fractures). Stratigraphic heterogeneity, only type considered here, indicates the degree of interbedding between high and low permeability layers. It controls phase flow parameters such as porosity, absolute permeability, relative permeability and capillary pressure curves. Numerical models have been developed and applied to synthetic or natural storage sites to assess the impact of the spatial variability of these flow parameters<sup>2,7,8,9</sup>. For memory and computational time reasons these models cannot account for the multi scale spatial variability. Because of their complexity they also cannot be used for site performance and risk assessment studies. As in petroleum engineering full scale models of CO<sub>2</sub> storage sites need to be upscaled. Much of the upscaling approaches and techniques developed in reservoir modeling can be used for this purpose<sup>6</sup>. Nevertheless gravity is often neglected. Injected as a supercritical fluid, CO<sub>2</sub> is buoyant with respect to the site porewater, therefore gravity plays an important role in CO<sub>2</sub> injection and migration.

 $CO_2$  sequestration in deep saline aquifers, such like Utsira aquifer at the Sleipner site, is an option studied by many countries. Utsira is often idealized as a multilayered porous media consisting of high permeability sand layers separated periodically by low permeability shale

stratas<sup>2</sup>. Injected at the bottom of the aquifer  $CO_2$  migration towards the top of the aquifer may be approximated, far from the injection point, as a vertical transport process trough a vertical periodic layered porous column. This process is driven by three different types of forces: viscous, gravity, and capillarity. To authors knowledge no work has been published on upscaling of this transport problem. van Duijn et al.<sup>16</sup> studied the horizontal column case where gravity is absent and injection and capillarity are the only driving forces. The objective was to derive and validate with numerical simulations an effective saturation transport equation which accounts for capillary oil trapping at the microscale during water-drive in an oil reservoir. When gravity is added, *i.e.* the column is vertical and filled with a light phase (CO<sub>2</sub>) and a dense phase (water), upscaling is expected to become a much more complex task.

In this paper we present an upscaled model for the buoyant migration of a  $CO_2$  plume in a vertical column filled with a periodically layered porous medium<sup>13</sup>. Capillarity and injection are neglected. We show that the upscaled  $CO_2$  saturation transport equation is a Buckley Leverett equation with gravity. The upscaled flux functions must be determined numerically and we propose two analytical approximations. Finally the validity of the capillary free upscaled model is studied by means of numerical experiments and the saturations obtained with numerical and analytical flux functions are compared and discussed.

#### **2 DYNAMICS**

In a vertical column filled with a heterogeneous porous medium the migration of  $CO_2$  plume is described by the Buckley Leverett equation with gravity :

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial z} \left( F\left(z, S\right) \right) = 0 \tag{1}$$

where F(z,S) = k(z)f(S) is the gravity flux and  $f(S) = \frac{k_{rg}(S)k_{rw}(S)}{k_{rg}(S) + Mk_{rw}(S)}$ . k(z) is the

absolute permeability, M the mobility ratio and  $k_r$  the relative permeability (index g stands for CO<sub>2</sub> and w for water), given by Brooks Corey model in our case.

This equation has been studied, from a physical and/or numerical point of view, by different authors. Recently, for instance, Sillin et al.<sup>15</sup> analyzed the vertical motion of a gas plume by means of travelling-wave solutions and proposed their method to study  $CO_2$  leaks from deep geological formations. It is important to emphasize that the bell shaped of the flux function (Fig. 1) leads to a gas plume migration described as a sequence of shock and rarefaction waves at the top and the bottom of the plume (Fig. 1). This sequence depends strongly on the relative permeabilities and on the initial plume saturation distribution.

Very few work has been done on the heterogeneous porous medium case. Among the few authors we can cite, for instance Kaasschieter<sup>12</sup> who studied extensively, from a mathematical point of view, the case of a permeability discontinuity. Recently Hayek et al.<sup>10</sup> analyzed the vertical motion of a  $CO_2$  plume in a layered porous medium in 1D and in 2D. They showed that the dependency of the gravity flux function with the absolute permeability leads to a

saturation discontinuity at the interface between a low and a high permeability layer. When, for instance, the plume migrates from a high to a low permeability layer flux continuity cannot be verified at the layers interface over the entire range of saturation (Fig.2). If the plume saturation is such that continuity is not verified, low saturation  $S_1$  (Fig. 2), saturation will increase on the high permeability side of the interface until it reaches a saturation value, high saturation  $S_1$  (Fig. 2), such that flux continuity can be verified and CO<sub>2</sub> will enter into the low permeability layer with a saturation value  $S_2^*$ . This accumulation process is illustrated on Fig. 3 which shows the vertical migration of a plume injected at the bottom of a vertical column filled with a periodic layered porous medium. The figure shows also that the accumulation occurs only under the first low permeability layer. If injection is considered and the geometry is 2D Hayek et al. <sup>10</sup> showed that, as the injection flowrate decreases with elevation the flux function also decreases; therefore flux continuity condition at each interface leads to an accumulation observed at the Sleipner site<sup>4</sup>.

When the wettability of the medium, which describes the relative preference of a rock to be covered by a certain phase, is taken into account the relative permeability depends also on the nature of the layer. This dependency is expressed through the pore size index in Brooks Corey Law. Three types of wettability can be distinguished: water-wet (WW), oil-wet (OW), or gaswet (GW), and intermediate-wet (IW). Hayek et al.<sup>11</sup> showed that the plume migration process and the saturation distribution depends closely on the wettabilities of the high and low permeability layers, as illustrated on Fig. 4. This figure shows that, depending on the layers wettabilities, low permeability layer may be, either, depleted or enriched in CO<sub>2</sub>. Consequently if hysteresis is taken into account, as in Doughty's work<sup>8</sup>, the wettability of the layers may have an important impact on saturation history in each layer and finally on carbon trapping during the post injection period<sup>9</sup>.

#### **3 UPSCALING**

We consider a vertical column filled with a periodic layered porous medium made up of low and high permeability layers. Without any loss of generality we assume that the layers have the same thickness  $\delta$ . The absolute permeabilities of the low and high permeability layers are  $k_{-}$  and  $k_{+}$  respectively. The column length *H* is supposed to be much greater than  $\delta$ , and the small parameter  $\varepsilon = \delta/H$  is  $\varepsilon \ll 1$ . In a high permeability layer Eq.(1) reads

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial z} \left( F_{+} \right) = 0 \tag{2}$$

where  $F_{+}(S) = k_{+}f(S)$  is the flux in the high permeability layer. In the low permeability layer

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial z} \left( F_+ \right) = 0 \tag{3}$$

where  $F_{-}(S) = k_{-}f(S)$ . The flux continuity at the interface between two layers implies

$$F_{+}\left(S_{\text{int},+}\right) = F_{-}\left(S_{\text{int},-}\right) \tag{4}$$

where  $S_{int+}$  and  $S_{int-}$  are the saturation values on each side of the interface.

To upscale the model we adopt the homogenization procedure introduced initially by Bensoussan et al <sup>3</sup> for periodic structures and applied to multiphase flow problems in periodic porous media by many authors. More precisely we follow in this work the modelling approach of van Duijn et al.<sup>16</sup>, discussed in the introduction. In our problem the small parameter is  $\varepsilon$ . see Mouche et al.<sup>13</sup> for the computational details. The upscaled saturation is defined as  $\overline{S} = (S^0_+ + S^0_-)/2$  and the upscaled transport equation is a Buckley Leverett equation with gravity

$$\frac{\partial \overline{S}}{\partial t} + \frac{\partial \overline{F}(\overline{S})}{\partial z} = 0$$
<sup>(5)</sup>

 $\overline{F}$  is the upscaled flux. It satisfies the flux continuity condition

$$F_{+}(S_{+}^{0}) = F_{-}(S_{-}^{0}) = \overline{F}(\overline{S})$$
(6)

where  $S^0_{\pm}$  are the zeroth order terms of the  $\varepsilon$  expansion of the saturations  $S_{\pm}$ .

A permeability ratio  $k_{-}/k_{+} = 0.3$  is considered. The fluid and relative permeabilities parameters values are given in Mouche et al.<sup>13</sup>. These authors showed that flux continuity cannot be verified for the whole range of  $S_{+}^{0}$  values but only on two segments:  $0 \le S_{+}^{0} \le S_{1}$  and  $S_{2} \le S_{+}^{0} \le 1$ . The two saturations  $S_{1}$  and  $S_{2}$  are given by the relationship  $F_{+}(S_{1}) = F_{+}(S_{2}) = F_{-}(S_{M})$  where  $S_{M}$  is the saturation at which function f is maximum. This constraint defines two ranges of upscaled saturation  $0 \le \overline{S} \le \overline{S}_{1}$  and  $\overline{S}_{2} \le \overline{S} \le 1$  where  $\overline{S}_{1} = (S_{1} + S_{M})/2$  and  $\overline{S}_{2} = (S_{2} + S_{M})/2$  with  $F_{+}(\overline{S}_{1}) = F_{+}(\overline{S}_{2}) = F_{-}(S_{M})$ . Therefore upscaled saturations lying between  $\overline{S}_{1}$  and  $\overline{S}_{2}$  do not exist (Fig. 5).

The upscaled flux function must be computed numerically for each permeability ratio  $k_{-}/k_{+}$ . Nevertheless two analytical approximations of this function can be proposed as follows. Let us write  $S_{-} = \overline{S} + \delta \overline{S}$  and  $S_{+} = \overline{S} - \delta \overline{S}$ , then the flux continuity, Eq.(6), may be written  $k_{+}f(\overline{S} + \delta \overline{S}) = k_{-}f(\overline{S} - \delta \overline{S})$  and the function f may be expanded up to the second order in  $\delta \overline{S} : f(\overline{S} \pm \delta \overline{S}) \simeq f(\overline{S}) \pm \delta \overline{S}f'(\overline{S}) + \frac{1}{2}\delta \overline{S}^{2}f''(\overline{S})$ . Eliminating  $\delta \overline{S}$  leads to a first order upscaled flux functions  $\overline{F}(\overline{S}) = K_{H}(k_{+},k_{-})f(\overline{S})$ , where  $K_{H}(k_{+},k_{-})$  is the harmonic mean of the permeabilities of the low and high permeability layers, and to a second order flux function that can be found in Mouche et al.<sup>13</sup>

The upscaled fluxes computed numerically and obtained from the first and second order approximations are plotted on Fig. 5. As expected the second order gives a better approximation of the upscaled flux for saturations not too close of  $\overline{S}_1$  and  $\overline{S}_2$ , and is above the exact flux, particularly in the neighbourhood of  $\overline{S}_1$  and  $\overline{S}_2$ . Inversely the first order is below the exact flux function. None of the approximations restitute the curvature of the upscaled flux in the neighbourhoods of  $\overline{S}_1$  and  $\overline{S}_2$ .

We compare now the upscaled model with the small scale model. Three upscaled flux functions are considered : the exact flux function, obtained numerically, and the first order and second order approximations, discussed precedently. All the models are solved analytically and the solutions are exact, see Hayek et al.<sup>11</sup>. The small parameter  $\varepsilon$ , ratio of the layer thickness on the column height is set to 1/50. CO<sub>2</sub> saturation is imposed at the bottom of the column, z = 0, and the top, z = 1, is a zero flux boundary.

The saturation profiles before the CO<sub>2</sub> plume reaches the top of the column and after it has reached the top are displayed in Fig. 6. The exact upscaled saturation distributions fit perfectly well with the cell averaged solution. These two distributions are described by a shock between  $\overline{S} = 0$  and  $\overline{S} = \overline{S'_1}$  and a rarefaction wave between  $\overline{S} = \overline{S'_1}$  and  $\overline{S} = \overline{S_1}$ , where  $\overline{S'_1}$  is shown on Fig. 5. These saturations describe the convex hull of the low saturation branch of the exact upscaled flux function (Fig. 5). The saturation distributions computed with the first and second order fluxes, called first and second order saturation distributions, are described by shocks only and they travel faster than the "exact" shock, and the "second order" shock travels faster than the "first order" shock. This is explained by Fig. 5 which shows that: i) the convex hull of the low saturation branch of the exact flux function is made up of a straight line between  $\overline{S} = 0$  and  $\overline{S} = \overline{S'_1}$  and by the flux function between  $\overline{S} = \overline{S'_1}$  and  $\overline{S} = \overline{S_1}$ ; ii) the convex hulls of the low saturation branches of the first and second order flux functions are straight lines between  $\overline{S} = 0$  and  $\overline{S} = \overline{S_1}$ ; iii) the slope of the straight line describing the "second order" convex hull is greater than that describing the "first order" convex hull. Let us recall that the shock velocity is proportional to this slope.

Once the plume has reached the top of the column CO<sub>2</sub> starts to accumulate below the top, as shown on Fig. 6. Again the exact upscaled distributions, computed with the exact upscaled flux function, fit perfectly well with the cell averaged solution. Now saturation distributions depend both of the low and the high saturation branches of the flux functions (Fig. 5). The distributions are described by a rarefaction wave between  $\overline{S} = S_{rg}$ , at the top of the column where the flux is zero, and  $\overline{S} = \overline{S'_2}$ , and a reflected shock between  $\overline{S} = \overline{S'_2}$  and  $\overline{S} = \overline{S_1}$  at the bottom of the column. These saturations describe the concave hull of the flux function between  $\overline{S} = \overline{S_1}$  and  $\overline{S} = 0$  (Fig. 5). This concave hull is made up of the flux function between  $\overline{S} = 1$  and  $\overline{S} = \overline{S'_2}$  and of the straight line between  $\overline{S} = \overline{S'_2}$  and  $\overline{S} = \overline{S_1}$ . Again the "second order" reflected shock travels faster than the "first order" one. This is easily explained by the concave hulls of the first order and second order fluxes.

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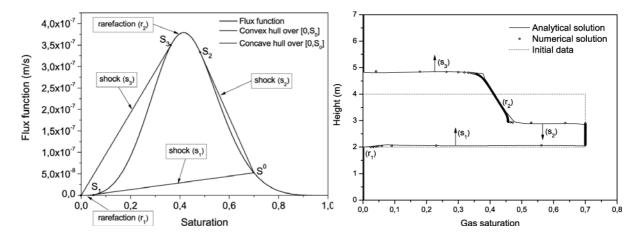


Figure 1:  $CO_2$  plume migration in a vertical column filled with a homogeneous porous medium: (left) convex and concave hulls for a plume of initial saturation  $S_0$ ; (right) analytical and numerical solutions at a short time.

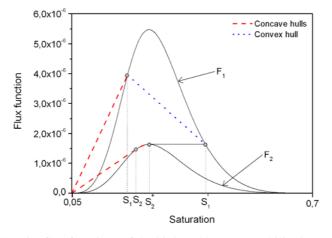


Figure 2 : Gravity flux functions of the high and low permeability layers (resp. F<sub>1</sub> and F<sub>2</sub>).

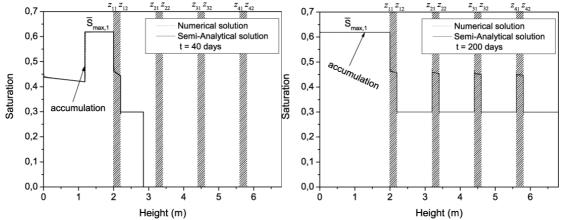


Figure 3 : CO<sub>2</sub> migration in a vertical column filled with a periodic layered porous medium. Numerical and semi-analytical solutions at (left) short time (40 days) and (right) long time (200 days).

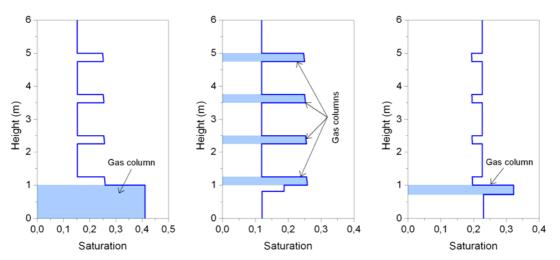


Figure  $4 : CO_2$  migration in a vertical column filled with a periodic layered porous medium : low permeability and high permeability layers are respectively : both intermediary wet (left), water wet and gas wet (center), gas wet and water wet (right).

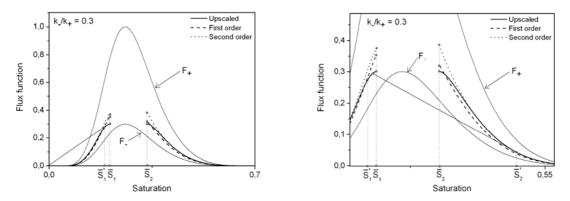


Figure 5 : Upscaled, first and second order gravity flux functions (left) convex hull and (right) concave hull

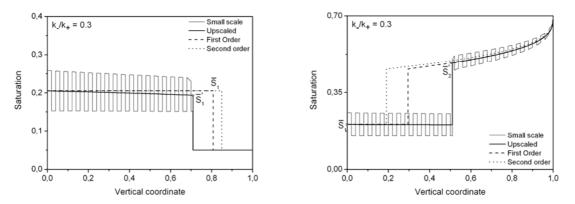


Figure 6 : Saturation distributions before (left) and after (right) the plume reaches the top of the column