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Comparison of Ross' Capillary Barrier Diversion Formula with Detailed Numerical Simulations

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Abstract

Ross (1990) developed an analytical relationship to calculate the diversion length of a tilted fine-over-coarse capillary barrier. Oldenburg and Pruess (1993) compared simulation results using upstream and harmonic weighting to the diversion length predicted by Ross' formula with mixed results; the qualitative agreement is reasonable but the quantitative comparison is poor, especially for upstream weighting. The proximity of the water table to the fine-coarse interface at breakthrough is a possible reason for the poor agreement. In the present study, the Oldenburg and Pruess problem is extended to address the water table issue. When the water table is sufficiently far away from the interface at breakthrough, good qualitative *and* quantitative agreement is obtained using upstream weighting.

I. Introduction

Capillary barriers, consisting of tilted fine-over-coarse layers under unsaturated conditions, have been suggested as a means to divert water infiltration away from sensitive underground regions. The capillary diversion formula of Ross (1990) (Steenhuis et al.,1991 and Stormont, 1995 present additional variations) is of particular interest because it can be easily used in capillary barrier design and evaluation. Oldenburg and Pruess (1993) compared TOUGH2 (Pruess, 1991) simulation results using upstream and harmonic weighting with Ross' formula; the results were mixed. While the comparison is reasonable qualitatively, the quantitative agreement is generally poor, especially for upstream weighting. A reason that has been proposed for this poor agreement is the proximity of the water table (Pruess, private communication, 1994). In Ross' derivation, the fine-coarse interface is assumed to be infinitely far away from the water table. In Oldenburg and Pruess (1993), the water table is only a few meters below the interface when breakthrough occurs. In order to address the water table proximity question, the Oldenburg and Pruess (1993) model is extended in the present study to allow for different initial water table locations. The applicability of upstream weighting to transient unsaturated flow conditions including capillary barrier behavior is also discussed.

While comparison of Ross' diversion equation with numerical modeling results is of interest, it must be kept in mind that capillary barrier leakage and breakthrough involve complicated unsaturated flow phenomena including fingering (Hill and Parlange, 1972; Glass et al., 1989a,b,c) as discussed by Oldenburg and Pruess (1993). Fingering phenomena are not treated in the analytical solution of Ross or in the TOUGH2 numerical code at present. In addition, heterogeneities and their spatial distribution may have a significant impact on the diversion length of tilted capillary barriers (Ho and Webb, 1997), which are not included in Ross' expression. Therefore, while comparison of Ross' expression with numerical results is of interest, comparison of modeling approaches to actual data is also needed.

II. Ross' Capillary Barrier Diversion Formula

Ross (1990) developed an analytical relationship to calculate the diversion length of a tilted fine-over-coarse capillary barrier with constant infiltration, assuming that the upper boundary (infiltration surface) and the lower boundary (water table) are far away from the fine-coarse interface. The only flow in the system is due to the infiltration. The analysis assumes steady-state conditions and defines breakthrough from the fine to the coarse layer as the occurrence of downward flow through the coarse layer equal to the infiltration rate. This assumption, along with the infiltration surface boundary condition, allows one to calculate the vertical relative permeability in the fine soil at breakthrough and,

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therefore, the horizontal flow in the fine layer. This horizontal flow is equal to the total amount of water diverted up until breakthrough

$$Q_{max} = K_s \tan \phi \int k_r \, d\psi \tag{1}$$

where ϕ is the angle of the fine-coarse interface with respect to horizontal. If the relative permeability is given by the quasi-linear function

$$k_r = e^{\alpha \psi} \tag{2}$$

where α is the sorptive number and ψ is the moisture potential ($\psi = P_c / \rho g$), then the equation reduces to a closed form solution

$$Q_{max} = K_s \frac{\tan \phi}{\alpha} \left[\left(\frac{q}{K_s^*} \right)^{\alpha/\alpha^*} - \frac{q}{K_s} \right] \tag{3}$$

where the starred value refers to the coarse layer parameter. For constant infiltration, the capillary diversion length is simply the total water diverted by the capillary barrier divided by the infiltration rate

$$L = K_s \frac{\tan \phi}{q \alpha} \left[\left(\frac{q}{K_s^*} \right)^{\alpha/\alpha^*} - \frac{q}{K_s} \right] \tag{4}$$

where L is the horizontal distance. Equation (1) above is general and can be used with any relative permeability function. Equations (3) and (4) are derived from equation (1) using the quasi-linear relative permeability function. The diversion length can be evaluated numerically for other relative permeability expressions such as van Genuchten (1980) as discussed by Webb (1997).

III. TOUGH2 Numerical Simulations

Oldenburg and Pruess (1993) analyzed a two-dimensional tilted fine-over-coarse capillary barrier with a water table and vertical infiltration using TOUGH2 (Pruess, 1991). For consistency with the Ross derivation, TOUGH2 was modified to include the quasi-linear wetting-phase relative permeability function discussed earlier. A sketch of the capillary barrier problem is given in Figure 1; properties and problem parameters are summarized in Table 1. A fine layer 50 m thick overlies a coarse layer 10 m thick; the layers are tilted at a 5° angle with respect to horizontal. Infiltration occurs at the top of the fine layer at a constant rate of 0.60 m/year, and a water table is specified at 59 m along the left boundary. For the conditions summarized in Table 1 ($\alpha = 0.1$ m^{-1}; $\alpha^* = 4.0$ m^{-1}), the predicted capillary diversion length from Ross (1990) is 39.3 m.

The discretization employed by Oldenburg and Pruess (1993) consisted of thirty rows each 2 m high with varying column widths. The column width was 4 m for the first 80 m downdip which increased thereafter. A higher resolution grid was examined between 32 and 80 m downdip using 2 m wide columns. The results from the original grid and the higher resolution grid are essentially the same.

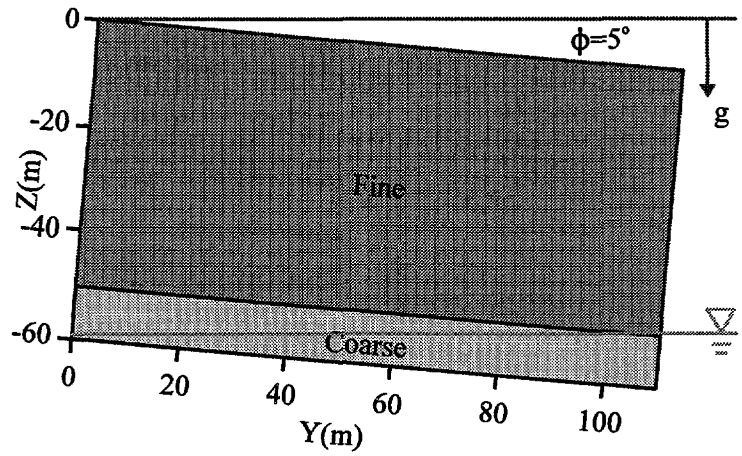


Figure 1
Comparison Problem Schematic
(after Oldenburg and Pruess, 1993)

Table 1
Original Problem Parameters

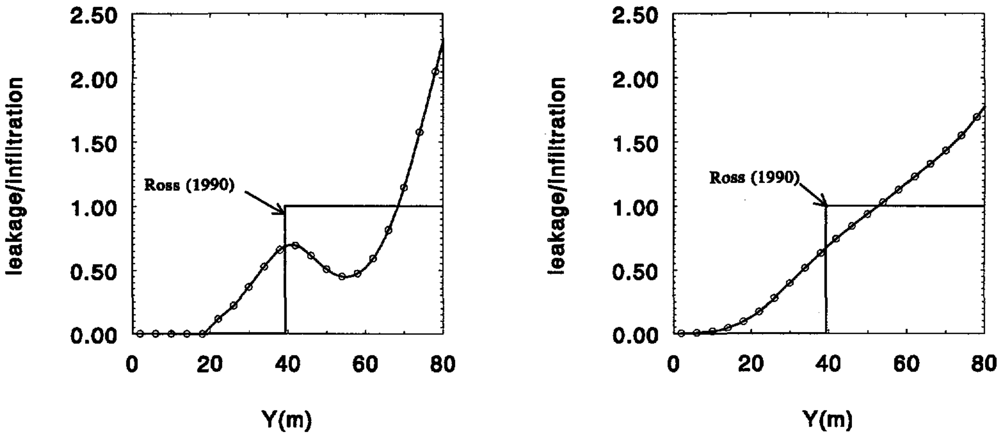
	Upper Layer (Fine)	Lower Layer (Coarse)
Thickness	50 m	10 m
Length	750 m	750 m
Permeability	10^{-13} m^2	2 x 10^{-13} m^2
Porosity	0.30	0.40
Relative Permeability	$k_r = e^{\alpha\psi}$; $\alpha = 0.1$ m^{-1}	$k_r = e^{\alpha^*\psi}$; $\alpha^* = 4.$ m^{-1}
Capillary Pressure	$P_c = - 10^6 (1.-S_l)$	$P_c = - 10^6 (1.-S_l)$

Boundary Conditions

Left Side	No flow.
Right Side	No flow.
Top	Constant Infiltration rate (0.60 m/year).
Bottom	Horizontal water table with a depth of 59 m at left boundary.

The results from the capillary barrier simulations are presented as a ratio of the leakage past the fine-coarse boundary divided by the infiltration rate. A value of zero shows complete diversion of the infiltrating water, while a value of 1.0 means no diversion. The ratio should increase with distance downdip until breakthrough occurs, which is defined as a ratio of 1.0. Values higher than 1.0 are expected further downstream when the diverted water flows into the coarse layer.

Oldenburg and Pruess (1993) investigated two different numerical weighting schemes for the permeability-mobility product ($k\ k_r / \mu$). The differences in the two schemes illustrate some of the complexities associated with unsaturated flow modeling. Harmonic weighting, which considers upstream and downstream parameters, is appropriate for steady-state one-dimensional flow without phase change or phase propagation based on flux conservation. However, for transient conditions involving phase propagation, flux conservation is not applicable, and upstream weighting is more appropriate. Upstream weighting, which only uses the upstream parameters, is numerically much more efficient and robust than harmonic weighting.



(a) Harmonic Weighting

(b) Upstream Weighting

<u>Figure 2</u>
TOUGH2 Leakage/Infiltration Ratio Results

The use of harmonic weighting for transient unsaturated flow can lead to large errors and upstream weighting is preferable (Aziz and Settari, 1979; Tsang and Pruess, 1990). In fact, harmonic weighting can lead to unphysical results in transient analyses of tilted capillary barriers such as the complete saturation of the upper fine layer without any leakage or flow into the lower coarse layer. Upstream weighting results are predominantly shown in the present paper.

The leakage/infiltration ratio as a function of distance downdip is given in Figure 2 for the Oldenburg and Pruess (1993) problem with coarse and fine layer sorptive numbers of 4.0 m^{-1} and 0.1 m^{-1}, respectively. This ratio is shown for harmonic and upstream weighting as calculated by the present author; the results are essentially the same as those in Oldenburg and Pruess (1993) The behavior of the leakage/infiltration ratio is significantly different for the two weighting schemes. The leakage/infiltration ratio using harmonic weighting shows an initial breakthrough at about 40 m. This ratio decreases slightly after this location because some of the water has flowed into the coarse layer. The ratio then increases again. In contrast, for upstream weighting, the ratio increases monotonically with distance. The agreement between the numerical results and Ross' formula is mixed. The comparison is reasonable qualitatively because the breakthrough location is in general agreement. However, the quantitative agreement is poor, especially for upstream weighting, because the leakage/infiltration ratio behavior is considerably different than the Ross (1990) model results for both numerical weighting schemes.

As discussed earlier, one reason that has been proposed for the poor agreement between the numerical simulations and Ross formula is the proximity of the water table. In Ross' derivation, the fine-coarse interface is assumed to be infinitely far away from the water table, while the water table is only a few meters below the interface when breakthrough occurs in the Oldenburg and Pruess (1993) problem. If the water table is near the fine-coarse interface, the moisture content and relative permeability of the coarse material will increase due to the added moisture from the capillary fringe, and the capillary pressure will be reduced. The net effect is to decrease the contrast between the fine and the coarse layers which will reduce the capillary barrier effectiveness. In order to address the water table proximity question, the initial water table location is varied in the present investigation.

In order to perform the modeling with different water table locations, the model domain was expanded. The depth of the coarse layer was increased from 10 meters to 50 meters for a total model depth of 100 meters. The vertical discretization was kept constant at 2 meters similar to Oldenburg and

Pruess (1993), resulting in 50 elements in the z-direction. In addition, since the location of breakthrough is expected to change with water table depth, the y (downdip) discretization was kept at a constant value of 4 meters for a total distance of 800 meters (Oldenburg and Pruess had a total distance of 750 meters) with a total of 200 elements in the y-direction. Therefore, the total grid consisted of 10,000 elements.

The standard version of TOUGH2 (Pruess, 1991) employs a full two-phase treatment of unsaturated flow with conservation equations for both the air and water phases. A Richards' equation treatment, which only considers water movement, is also available (Pruess and Antunez, 1995). As shown by Webb (1996), the full two-phase treatment and the Richards' equation results are essentially the same for the Oldenburg and Pruess capillary barrier problem, and the Richards' equation solution time is only 1/10 of the full two-phase treatment. Therefore, the Richards' equation version has been used in the present study including Figure 2 above. The conjugate gradient solvers of Moridis and Pruess (1995) have also been used.

The water table in Oldenburg and Pruess is at z=-59 meters along the left edge of the domain, or 9 meters (m) below the fine-coarse interface. In the present study, water table locations of 5, 9, 13, 19, 29, 39, and 49 m below the fine-over-coarse interface have been considered with upstream weighting. The problems were run in two parts. Initial conditions were established by running a false transient to steady-state with the water table but without infiltration. The infiltration transient was then performed by using the calculated initial conditions and applying the infiltration uniformly along the top surface. The bottom boundary pressures remained constant during the transient, which provided a sink for the infiltrating water that breaks through. The simulation was run until steady-state conditions were achieved. Leakage across the fine-coarse boundary was then compared to the infiltration rate to determine the leakage/infiltration ratio.

Figure 3 compares the results from TOUGH2 and Ross' (1990) formula for the various initial water table depths. For an initial water table elevation 5 m below the fine-coarse interface, the leakage/infiltration ratio increases monotonically, reaching a maximum value of about 1.7 at 38 m. For an initial water table elevation 9 m below the interface, the leakage/infiltration ratio increases monotonically, and the ratio reaches a maximum value approaching 2.0 at 82 m. These results are similar but not exactly the same as given by Oldenburg and Pruess (1993). Small differences between the two results are expected due to the expanded computational domain employed in the present simulations and the different treatment of unsaturated flow. For an initial water table 13 m below the interface, the leakage/infiltration ratio again increases monotonically, although the ratio shows a tendency to "flatten out" slightly at intermediate distances. The peak ratio is about 2.0 at 126 m downdip.

Results for initial water table depths of 19 m, 29 m, 39 m, and 49 m are also shown in Figure 3. As the initial water table depth increases, three regions are evident. They are 1) initial increase in leakage/infiltration ratio, 2) leakage/infiltration plateau at a value of 1.0, and 3) increase in the ratio above 1.0 as the water table is approached. (The downdip distance corresponding to the intersection of the water table with the fine-coarse interface is simply the initial water table depth divided by tan 5°, or 0.0875.) For example, the leakage/infiltration ratio from 0 to 100 m is essentially the same for water table locations 19 m or more below the fine-coarse interface. The breakthrough location is similar to that predicted by Ross (1990) although considerably more diffuse due to the numerical behavior of upstream weighting (see, for example, Oran and Boris, 1987). The ratio then remains at a value of 1.0 until the water table is approached. The leakage/infiltration ratio then increases to a value of about 2.0 as water flows down to the water table in the capillary fringe region.

In summary, for initial water table depths of 13 m or less, the location of the water table significantly influences the initial behavior of the leakage/infiltration ratio; this range includes the original Oldenburg and Pruess (1993) problem specification of 9 m. For larger initial water table depths of 19 m or more, the initial leakage/infiltration ratio is not affected by the location of the water table.

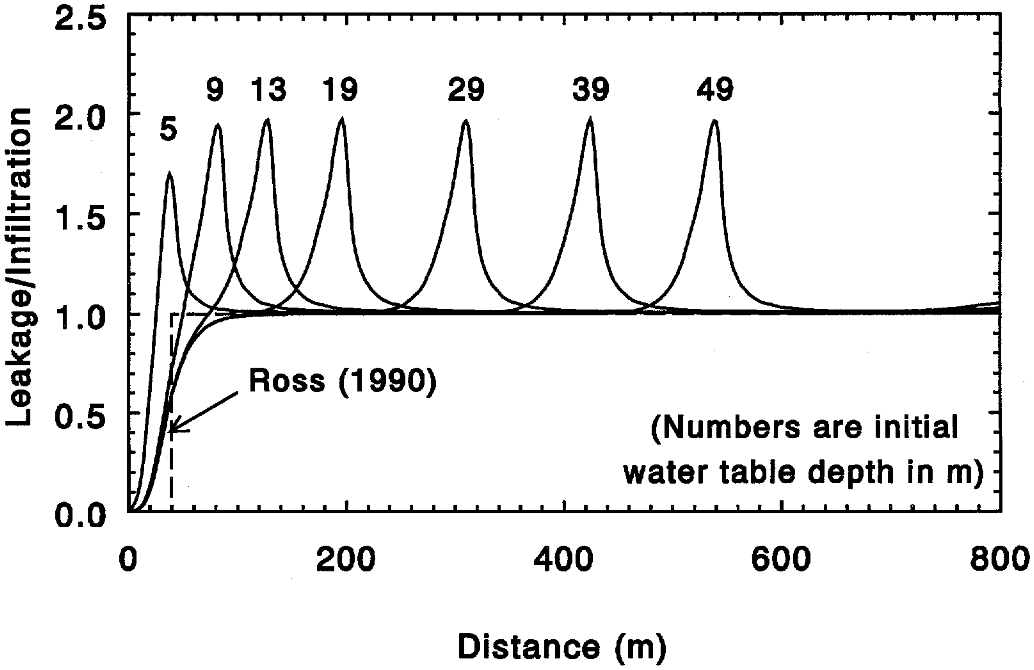


Figure 3
TOUGH2 Leakage/Infiltration Ratio Result
As a Function of Initial Water Table Depth

IV. Discussion and Conclusions

Results from numerical simulations using upstream weighting have been compared to Ross' tilted capillary barrier diversion formula for the Oldenburg and Pruess (1993) capillary barrier problem with variable water table locations. For a sufficiently deep water table, which is consistent with the assumption used by Ross (1990), the simulations are in good qualitative *and* quantitative agreement with Ross' capillary barrier diversion formula. For shallower water tables, including the Oldenburg and Pruess (1993) location, the results are significantly influenced by the water table. These results indicate that upstream weighting can accurately model capillary barrier behavior as evidenced by good agreement between the simulations and Ross' formula for the deeper water table locations.

These results are significantly different than Oldenburg and Pruess (1993). Oldenburg and Pruess concluded that while upstream weighting may describe the general behavior of capillary barriers, it is not able to model the details of capillary barrier flow; harmonic weighting is required to resolve the details of breakthrough. Their conclusion is based on the difference between their upstream weighting results and Ross' (1990) formula as shown in Figure 2. Their conclusion has significant implications in unsaturated flow modeling for capillary barriers. As mentioned earlier, upstream weighting is often required for transient unsaturated flow modeling. Therefore, according to Oldenburg and Pruess (1993), modeling of transient unsaturated flow in capillary barriers involves numerical compromises; while upstream weighting is often required for numerical efficiency and stability, it is not as accurate as harmonic weighting. As mentioned by Oldenburg and Pruess (1993), this compromise not only applies to engineered capillary barriers such as discussed in this paper, but it also has important implications for simulation of natural capillary barrier effects such as encountered in potential nuclear waste repositories.

In contrast, the present study has shown that the disagreement observed by Oldenburg and Pruess (1993) was significantly influenced by the proximity of the water table. If the water table is deep enough, which is consistent with the assumption made by Ross (1990), simulations using upstream weighting agree well with Ross' capillary barrier diversion formula. Based on the present results, upstream weighting *can* be used to accurately model transient unsaturated flow including capillary barrier behavior.

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V. Nomenclature

K_s	saturated hydraulic conductivity for fine layer
K_s^*	saturated hydraulic conductivity for coarse layer
k_r	relative permeability
L	horizontal diversion length
P_c	capillary pressure
q	infiltration rate
Q	total horizontal flux
S_l	liquid saturation
α	sorptive number for fine layer
α^*	sorptive number for coarse layer
ρ	fluid density
μ	viscosity
ϕ	angle of the fine-coarse interface with respect to horizontal
ψ	moisture potential

VI. References

Aziz, K., and T. Settari (1979) *Petroleum Reservoir Simulation*, Applied Science Publishers, London.

Ho, C.K., and S.W. Webb (1997) "The Effects of Heterogeneities on the Performance of Capillary Barriers for Waste Isolation," 1997 ICTCE Conference, St. Petersburg, FL.

Moridis, G., and K. Pruess (1995) *Flow and Transport Simulations Using T2CG1, A Package of Conjugate Gradient Solvers For the TOUGH2 Family of Codes*, LBL-36235, Lawrence Berkeley Laboratory.

Oldenburg, C.M., and K. Pruess (1993) "On Numerical Modeling of Capillary Barriers," *Water Resour. Res.*, Vol. 29:1045-1056.

Oran, E.S., and J.P. Boris (1987) Numerical Simulation of Reactive Flow, Elsevier, New York.

Pruess, K. (1991) *TOUGH2 - A General-Purpose Numerical Simulator for Multiphase Fluid and Heat Flow*, LBL-29400, Lawrence Berkeley Laboratory, May 1991.

Pruess, K., and E. Antunez (1995) "Applications of TOUGH2 to Infiltration of Liquids in Media with Strong Heterogeneity," in *Proceedings of the TOUGH Workshop '95*, K. Pruess, ed., pp. 69-76, LBL-37200, Lawrence Berkeley Laboratory.

Ross, B. (1990) "The Diversion Capacity of Capillary Barriers," *Water Resour. Res.*, 26:2625-2629.

Ross, B. (1991) "Reply", *Water Resour. Res.*, 27:2157 (see Steenhuis et al., 1991).

Steenhuis, T.S., J.-Y. Parlange, and K.-J.S. Kung (1991) "Comment on 'The Diversion Capacity of Capillary Barriers,' by Benjamin Ross," *Water Resour. Res.*, 27:2155-2156 (see Ross, 1991).

Stormont, J.C. (1995) "The Effect of Constant Anisotropy on Capillary Barrier Performance," *Water Resour. Res.*, 31:783-785.

Tsang, Y., and K. Pruess (1990) *Further Modeling Studies of Gas Movement and Moisture Migration at Yucca Mountain, Nevada*, LBL-29127, Lawrence Berkeley Laboratory.

van Genuchten, M.Th. (1980) "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils," *Soil Sci. Soc. Am. J.*, 44:892-898.

Webb, S.W. (1996) "Selection of a Numerical Unsaturated Flow Code for Tilted Capillary Barrier Performance Evaluation," SAND96-2271, Sandia National Laboratories.

Webb, S.W. (1997) "Generalization of Ross' Tilted Capillary Barrier Diversion Formula For Different Two-Phase Characteristic Curves," submitted to *Water Resources Research*.