

Upscaling unsaturated flow in binary porous media with air entry pressure effects

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[1] We consider flow in a porous medium containing coarse-textured inclusions with a low value of air entry pressure, embedded in a fine-textured background material having high entry pressure. During imbibition some air remains trapped in the inclusions, while during drainage the inclusions become drained only after the capillary entry pressure exceeds the pressure of the background material. These effects can only be reproduced by a two-phase flow model, and not by the Richards' equation. However, if an upscaled form of the Richards' equation with appropriately modified capillary and permeability functions is used, the results are in a reasonable agreement with the two-phase flow model.

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1. Introduction

[2] The flow of water and air in the vadose zone can be described either with a two-phase model or with a simplified model known as the Richards' equation. The latter approach is based on the assumption that the air phase is continuous, connected to the atmosphere, and much more mobile than water. Consequently, the air pressure in soil can be regarded as constant and equal to the atmospheric pressure. However, in porous media characterized by spatial variability of the air entry pressure, the air phase can lose its connectivity, giving rise to significant differences observed between the results of the two-phase model and the Richards' equation. Here we use the term air entry pressure in relation to both imbibition and drainage. We define it as the characteristic value of the capillary pressure above which the airflow is possible. The air entry pressure is included as a parameter in several analytical models for capillary pressure–saturation relationships [e.g., *Brooks and Corey*, 1964; *Rucker et al.*, 2005].

[3] The effects of entry pressure heterogeneity can be particularly important for media consisting of fine-textured background material with high entry pressure and disconnected, coarse-textured inclusions having low entry pressure. During imbibition the fine material around inclusions becomes fully saturated at a higher value of the capillary pressure than the coarse material. The air remaining in the isolated coarse regions is trapped since it cannot invade the fine material, unless the entry pressure is exceeded. A similar effect can also be observed when the background material is not fully saturated, but contains only a small amount

of air. In such a case the fine material can often be considered practically impermeable for air at the relevant time scale. On the other hand, during drainage the air can move through the fine material to the coarse regions only after the entry pressure of the fine material is exceeded. It means that the coarse regions remain fully saturated, even if the actual capillary pressure in the medium corresponds to a lower water saturation in the coarse material. Experimental evidence for such behavior can be found by *Vasin et al.* [2008]. These effects can be simulated with the full two-phase model, but not with the Richards' equation, which does not take into account the airflow, and consequently does not require the volume of water entering the system to be balanced with an equivalent volume of air leaving the system.

[4] If the number of heterogeneous regions is large, explicit representation of the heterogeneous structure on a numerical grid becomes impractical and upscaling methods have to be used. Upscaled models accounting for the non-wetting phase entry pressure were developed by *Mikelic et al.* [2002] and *van Duijn et al.* [2007] for one-dimensional layered media and by *Szymkiewicz et al.* [2011] for multi-dimensional media with coarse inclusions. This note is an extension of the latter work, written with two objectives. The first one is to emphasize the limitations of the standard Richards' equation for porous media showing a specific heterogeneity pattern with disconnected coarse inclusions. The second one is to present a preliminary evaluation of a modified upscaled form of the Richards' equation, which accounts for the apparent air entry pressure effects caused by heterogeneous structure.

2. Mathematical Models

[5] Our approach is based on the periodic homogenization method. For a more detailed presentation of the underlying assumptions and the derivation procedure the reader is referred to the papers of *Saez et al.* [1989] and *Lewandowska and Laurent* [2001] for the case without entry pressure and [*Szymkiewicz et al.*, 2011] for the case of entry pressure

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effects. The equation for large scale flow of fluid phase α [$\alpha = w$ (water) or a (air)] is similar to the equation used at the local (Darcy) scale:

$$\frac{\partial(\rho_\alpha^E \theta_\alpha^E)}{\partial t} - \nabla \cdot \left[\rho_\alpha^E \frac{\mathbf{k}_\alpha^E}{\mu_\alpha} (\nabla p_\alpha^E + \rho_\alpha^E \mathbf{g}) \right] = 0, \quad (1)$$

where the superscript E denotes effective (macroscopic) variables, ρ is density, θ is the volumetric phase content, \mathbf{k} is the phase permeability tensor, p is the phase pressure, and \mathbf{g} is the gravity vector.

[6] The upscaled model is based on the assumption of local capillary equilibrium, i.e., the pressures in each phase and the capillary pressure $p_c^E = p_a^E - p_w^E$ are constant within an assumed macroscopic representative elementary volume (REV) or periodic cell. Such conditions can be assumed to be appropriate if the parameter contrast between background and inclusion material is not too large. The water saturation and the phase permeabilities for each material region within REV are then computed from the local capillary functions for the assumed value of the macroscopic capillary pressure. The corresponding macroscopic porosity, phase contents, and saturations are calculated as follows: $\phi^E = w^B \phi^B + w^I \phi^I$, $\theta_\alpha^E = w^B \theta_\alpha^B(p_c^E) + w^I \theta_\alpha^I(p_c^E)$, and $S_\alpha^E = \theta_\alpha^E / \phi^E$, where the superscripts B and I denote the background and inclusions, respectively, and w is the volume fraction of the material. Once the local distribution of phase permeabilities is known, the effective permeability tensor can be obtained by solving the so-called cell problem for each phase, which corresponds to steady single-phase flow with periodic boundary conditions and with the permeability configuration resulting from the fluid configuration at a given capillary pressure [e.g., Saez *et al.*, 1989; Szymkiewicz *et al.*, 2011]. The effective permeability for each value of the capillary pressure can be also computed using simpler methods, provided that they take into account the information about the connectivity of the materials [e.g., Knudby *et al.*, 2006; Svierecki, 2010]. In the following examples we used a Maxwell-type approximate formula suitable for media containing uniformly aligned ellipsoidal inclusions, well-separated from each other [e.g., Milton, 2002; Torquato, 2002]:

$$k_{\alpha,ii}^E = k_\alpha^B + \frac{w^I (k_\alpha^I - k_\alpha^B)}{1 + w^B d_i (k_\alpha^I - k_\alpha^B) / k_\alpha^B}, \quad (2)$$

where d_i is the depolarization factor for i th spatial direction. For 2-D ellipses $d_1 = \frac{a_2}{a_1 + a_2}$ and $d_2 = \frac{a_1}{a_1 + a_2}$, where a_i is the length of the ellipse axis parallel to i th direction.

[7] In principle, the approach described above can be used to obtain the macroscopic capillary pressure–saturation relationship for the whole range of capillary pressure values. However, for media with disconnected coarse-textured inclusions it is applicable only in the range of the capillary pressures above the entry pressure of the fine background material p_e^B , with the corresponding threshold water saturation and volumetric water content equal to $\theta_w^{E*} = w^B \phi^B + w^I \phi^I S_w^I(p_e^B)$ and $S_w^{E*} = \theta_w^{E*} / \phi^E$. During the imbibition the macroscopic water content cannot increase above a threshold value, because the air cannot escape from the inclusions to the fully saturated background material. The corresponding air saturation $S_a^{E*} = 1 - S_w^{E*}$ can be

regarded as the large-scale residual air saturation due to the entrapment of air in textural heterogeneities. Consequently, the effective permeability of the medium is also reduced with respect to its value at full water saturation, $k_{w,ij}^{E*} = k_{w,ij}^E (S_w^{E*}) < k_{w,ij}^E (S_w^E = 1)$.

[8] During the drainage from a fully water-saturated state the medium remains fully saturated and the permeability with respect to water is at its maximum value, until the capillary pressure exceeds p_e^B . Inclusions only drain after they have been reached by the draining front in the background, as air cannot access the inclusions before that. As soon as the air flowing through the background material encounters an inclusions, the values of water saturation and permeability rapidly drop to S_w^{E*} and k_w^{E*} , respectively. At the scale of a single REV this process is not instantaneous, but here we consider it as relatively fast in comparison to the overall time of flow. Thus, the upscaled functions show a discontinuity at the point p_e^B . As a result, a quasihysteresis is obtained in the upscaled hydraulic functions since in the range of capillary pressures below p_e^B they have different values for imbibition and drainage.

[9] In the following examples we compare the results obtained with several mathematical models. 2PH-FS denotes the fine-scale solution of the two-phase model, with explicit representation of the material heterogeneities. It is considered the reference solution since it is expected to give the most accurate results within the framework of assumed conceptual model of flow in porous media. 2PH-UPS is the upscaled version of the two-phase model, which accounts for the entry pressure effects [Szymkiewicz *et al.*, 2011]. RE-FS is the fine scale solution obtained with the Richards' model, while RE-UPS-1 corresponds to the Richards' equation upscaled using the standard approach, which does not take into account the entry pressure and produces a unique capillary and permeability functions in the range of water pressures above $-p_e^B$. Finally, RE-UPS-2 is the upscaled Richards' equation with hydraulic functions calculated according to the approach proposed by Szymkiewicz *et al.* [2011]. In the upscaled models we further distinguish between the effective permeability obtained from the periodic homogenization (H) and from the Maxwell-type formula (M). In order to minimize the influence of numerical errors, all equations were solved on the same numerical grid, although upscaled models are typically applied at much coarser grids than fine scale solutions.

3. Example 1

[10] The first example concerns quasi-1-D flow in a soil column (0.1 m by 1 m) with 10 periodically placed inclusions (0.05 by 0.05 m). Both materials are characterized by Brooks–Corey–Burdine hydraulic functions, with the same value of exponent $\lambda = 1.5$. In the fine background material the entry pressure is 3000 Pa and the absolute permeability is isotropic and equal to 10^{-11} m^2 , while for the coarse inclusions the values are 1000 Pa and 10^{-10} m^2 , respectively. In each material the porosity is 0.4 and the residual phase saturations are zero. Due to isotropic local geometry the upscaled permeability is a scalar. The effective absolute permeability values obtained from periodic homogenization and from the Maxwell-type approximation are 1.54×10^{-11} and $1.51 \times 10^{-11} \text{ m}^2$, respectively. At the

threshold saturation ($p_c = 3000$ Pa) the values of permeability for the water phase are 5.83×10^{-12} and 6.00×10^{-12} m², respectively. As the differences are slight, only the results for periodic homogenization are reported here. The density, viscosity, and compressibility of each fluid corresponds to the temperature of 20°C. Initially, the whole column is fully water saturated, with hydrostatic distribution of the water pressure from 0 at the top to 9810 Pa at the bottom (all pressure values are relative to the atmospheric pressure). The top of the column is assumed to be impermeable for water, while air is kept at constant atmospheric pressure $p_a = 0$. At the bottom of the column the air pressure has the same constant value $p_a = 0$, while the water pressure varies. During the first hour it decreases linearly from the initial value to zero, which is maintained for the next 3 h. Then it is linearly increased, reaching the initial value of 9810 Pa for $t = 5$ h and remains constant for the rest of the simulation time. All numerical solutions were obtained on a uniform grid of 200 by 20 cells.

[11] Numerical simulations carried out for homogeneous medium without inclusions (results not shown here) showed a good agreement between the two-phase model and the Richards' model, while the presence of coarse inclusions leads to significant discrepancies between models. The distributions of water saturation obtained with fine scale models 2PH-FS and RE-FS can be compared in Figure 1 for two different simulation times, corresponding to the drainage

and upward infiltration stages, respectively. The evolution in time of the averaged water saturation in the domain is presented in Figure 2. According to the 2PH-FS solution the drainage starts later than for Richards' equation. In the former case, the water can be drained only when the background material becomes permeable to air, i.e., after the water pressure falls below $-p_e^B$. In the RE-FS simulation the drainage starts as soon as the entry pressure for the inclusions is exceeded. Figure 1 shows that according to the 2PH-FS model at the end of the drainage phase ($t = 3$ h) the inclusions located in the lower third of the column remain saturated since the water pressure here is between 0 and -3000 Pa, and the saturation of the background material does not allow for airflow. In contrast, RE-FS predicts drainage of two inclusions located in this zone, which means that the total amount of water retained in the medium is smaller.

[12] During the infiltration phase, the differences between the two-phase model and the Richards' equation become even more pronounced. According to the 2PH-FS solution a relatively large amount of air becomes trapped in the inclusions, without the possibility to escape, even after a long time (in real-life conditions the entrapped air would slowly dissolve in water, or move in the form of small bubbles, but these mechanisms are not included in the standard two-phase immiscible flow model). In contrast, air trapping is not present in the RE-FS solution, which does not

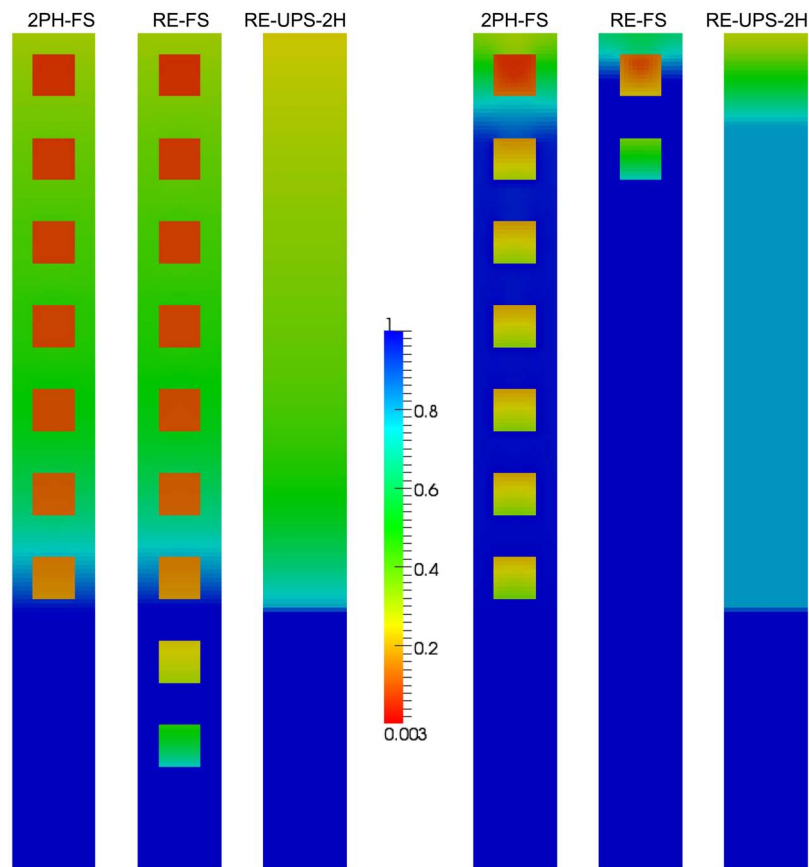


Figure 1. Example 1: Water saturation distribution. Left: $t = 3$ h, drainage, right: $t = 4$ h, imbibition. The different models are indicated on the top of the figures.

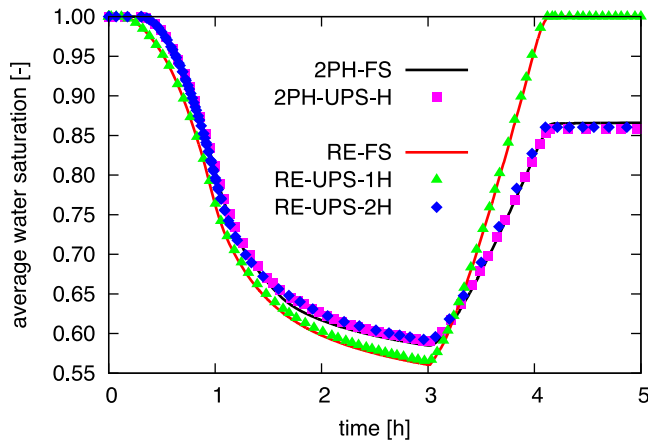


Figure 2. Example 1: Evolution of the average water saturation in the solution domain.

account explicitly for the airflow. Thus, RE-FS predicts a reversible process similar to the model representing a homogeneous medium, i.e., at the end of infiltration phase the initial state of full saturation is reached. In 2PH-FS solution the drainage-infiltration cycle is not reversible since air trapping in textural heterogeneities does not allow the medium to become fully saturated in the infiltration phase.

Note that each of the materials is characterized by the same set of hydraulic functions for infiltration and drainage, so the differences between drainage and wetting during the first cycle are solely due to macroscopic textural heterogeneities, not porescale phenomena.

[13] Figure 2 shows that RE-UPS-1H solution closely follows RE-FS solution, while 2PH-UPS-H is in good agreement with 2PH-FS. This confirms the validity of the homogenization approach applied in the framework of each of the two models. If the upscaled function accounting for the air entry effects are applied to the Richards' equation (RE-UPS-2H), the results are very close to the reference 2PH-FS solution and upscaled two-phase solution 2PH-UPS. This is further confirmed by Figure 1, where the average saturations obtained with RE-UPS-2H match well the nonuniform saturation distribution from 2PH-FS.

4. Example 2

[14] The second example concerns two-dimensional infiltration with gravity in a medium with randomly placed lenses of a uniform vertical dimension of 0.02 m and horizontal dimensions varying from 0.06 to 0.14 m, with the average of 0.089 m. The inclusions were placed at arbitrarily chosen points without following any particular statistic distribution pattern (see the upper right plot in Figure 3). The volumetric fraction of the lenses is $w^l = 0.165$. In this

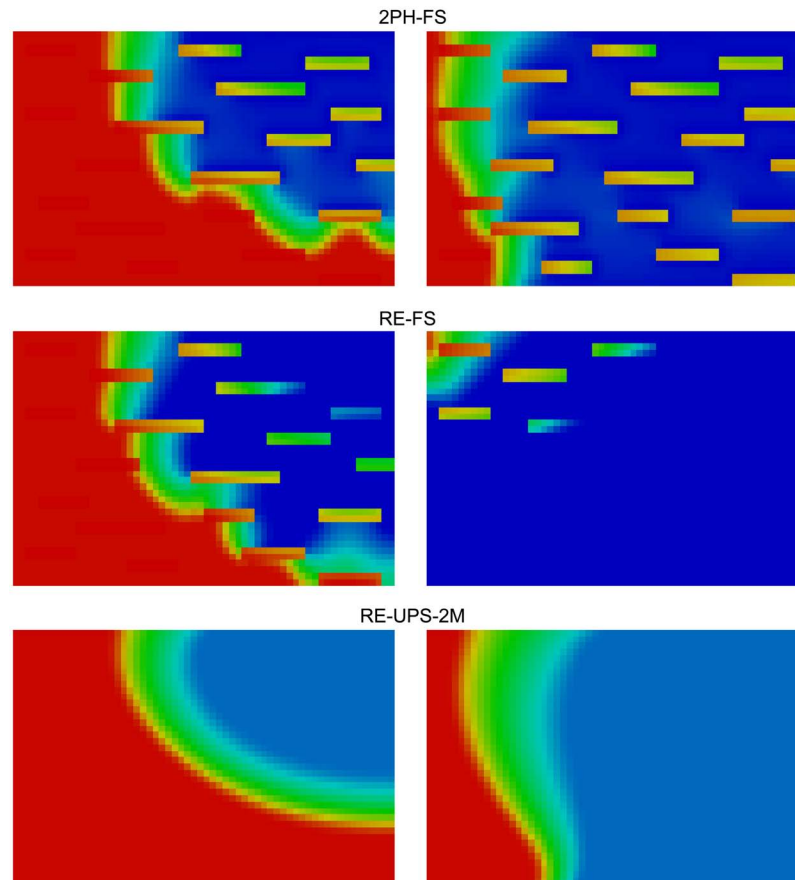


Figure 3. Example 2: Water saturation distribution. Left: $t = 0.1$ h, right: $t = 0.417$ h. The color scale is the same as in Figure 2.

case no representative elementary volume can be distinguished and the separation of scales is poor, which means that the assumptions underlying the upscaling approach of Szymkiewicz *et al.* [2011] are not fulfilled. The effective permeability was computed by solving the periodic boundary value problem for the whole domain. This yielded the values of the water permeability at the threshold saturation equal to $7.93 \times 10^{-12} \text{ m}^2$ in the horizontal direction and $4.14 \times 10^{-12} \text{ m}^2$ in the vertical direction. Equation (2) (for which we used the average lens dimensions) gave the corresponding values of 8.08×10^{-12} and $4.61 \times 10^{-12} \text{ m}^2$. The difference in vertical permeability, which appeared also for other values of the capillary pressure, is reflected in the infiltration rate as shown below. The initial condition was $p_w = -50,000 \text{ Pa}$ and $p_a = 0$. At the right hand part of the upper boundary ponded infiltration is enforced, with $p_w = 0$ and $p_a = 0$. The remaining part of the upper boundary is impermeable to water but permeable to air, with the air pressure equal to the atmospheric one ($p_a = 0$). The other boundaries are impermeable to both water and air. All numerical solutions were obtained on a uniform grid of 60 by 40 cells.

[15] The spatial distribution of the water saturation in the solution domain is shown in Figure 3 and the time evolution of the averaged water saturation—in Figure 4. The 2PH-FS solution predicts a smaller infiltration rate and smaller water content compared to the RE-FS solution. The comparison of various upscaled solutions show several interesting features. First, we note that the RE-UPS-1 solution is not sensitive to the choice of method of permeability estimation (periodic homogenization or Maxwell-type approximation) and is in a good agreement with RE-FS solution. Second, the RE-UPS-2 and 2PH-UPS solutions underestimate the infiltration rate with respect to the reference 2PH-FS solution, but predict similar final saturation in the domain. As it can be seen in Figure 3, the infiltration front moves more slowly according to the RE-UPS-2M solution than to the 2PH-FS model. Moreover, RE-UPS-2 and 2PH-UPS models are sensitive to the permeability upscaling technique, with the Maxwell formula yielding results closer to the reference solution. Third, for each method of permeability estimation we observe a discrepancy between the

respective RE-UPS-2 and 2PH-UPS solutions. It should be noted that a similar difference was observed for flow in homogeneous medium without inclusions. While the results are not shown here, this discrepancy practically disappeared if the air viscosity was reduced by an order of magnitude, indicating that viscosity effects are non-negligible in this case. Finally, we note that the results obtained with the RE-UPS-2 models are in better agreement with the reference solution than the results obtained with the 2PH-UPS models. This is due to the fact that in the RE-UPS-2 solutions the error introduced by neglecting the air viscosity partially compensates for the underestimation of the effective permeability.

5. Conclusions

[16] Numerical examples presented in this paper show that heterogeneities in the air entry pressure may significantly affect the applicability of the Richards' equation to model water flow in porous medium. If the medium contains disconnected coarse inclusions with an entry pressure lower than that of the background material, a considerable discrepancy is observed between the numerical results obtained with the two-phase model and the Richards' equation for both infiltration and drainage. This discrepancy can be reduced if the Richards' equation is solved at the macroscopic scale with appropriately upscaled capillary and conductivity functions, which take into account the entry pressure effects. While the second example showed a less-than-perfect performance of the proposed approach applied to more realistic medium structure with a poor separation of scales, the results were still closer to the two-phase model than the results obtained with the standard Richards' equation.

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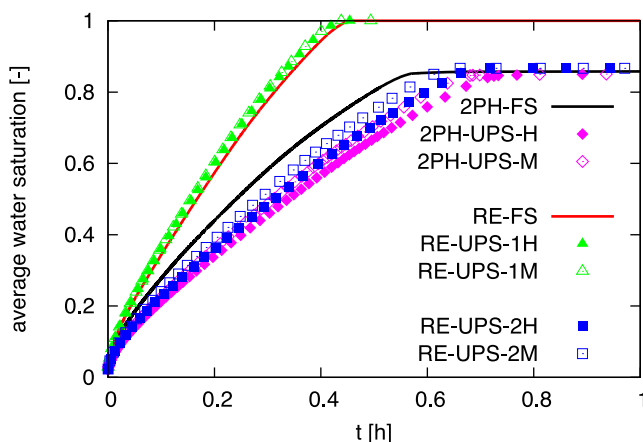


Figure 4. Example 2: Evolution of the averaged water saturation in the solution domain of Figure 3.

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