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in porous media: Theory and experiments.

Publications in peer reviewed scientific magazines

Ataie-Ashtiani, B., S.M. Hassanizadeh, M. Oostrom, M.A. Celia, and M. White, "Effective parameters for two-phase flow in a porous medium with periodic heterogeneities," *J. Contam. Hydrol.*, vol. **49**, pp. 87-109, 2001.

Ataie-Ashtiani, B., S.M. Hassanizadeh, and M.A. Celia, "Effects of heterogeneities on capillary pressure-saturation-relative permeability relationships," *Journal of Contaminant Hydrology*, vol. **56**, pp. 175–192, 2002.

Hassanizadeh, S.M., M.A. Celia, and H.K. Dahle, "Dynamic effect in the capillary pressure-saturation relationship and its impacts on unsaturated flow," *Agricultural Sciences*, **7**, pp. 69-71, 2002.

Ataie-Ashtiani, B., S.M. Hassanizadeh, O. Oung, F.A. Weststrate, and A. Bezuijen, "Application of numerical simulation in interpretation of two-phase flow experiment in a centrifuge," *Environmental Modelling and Software*, **18**, pp. 231-241, 2003.

Das, D.B., S.M. Hassanizadeh, B. Rotter B. Ataie-Ashtiani. "A numerical study of microheterogeneity effects on upscaled properties of two-Phase flow in porous media" accepted for publication in *Transport in Porous Media*, **56**, pp. 329-350, 2004.

H.K. Dahle, Celia, M.A., and S.M. Hassanizadeh, "Bundle-of-tubes model for calculating dynamic effects in the capillary pressure-saturation relationship," *Transport in Porous Media*, Vol. **58**, no. 1-2, 2005.

Oung, O. & Bezuijen, A. (2003) 'Calibration and validation of developed selective pore pressure transducers for used in model tests', accepted for publication in *Int. J. of Physical Modelling in Geotechnics*, 2004.

Manthey, S., S.M. Hassanizadeh, and R. Helmig, "Macro-scale dynamic effects in homogeneous and heterogeneous porous media," *Transport in Porous Media*, Vol. 58, no.1-2, 2005.

Oung, O., S.M. Hassanizadeh, and A. Bezuijen, "Two-phase flow experiments in a geocentrifuge and the significance of dynamic capillary pressure effect," *Journal of Porous Media*, to appear, 2005.

Conference proceedings and contributions to books and monographies.

Ataie-Ashtiani, B., S.M. Hassanizadeh, M. Oostrom and M.D. White, "Numerical simulation and homogenization of two-phase flow in heterogeneous porous media," in: *Groundwater Updates*, proceedings of the IAHR International Symposium on Groundwater, Sonic City, Japan, 8-10 May 2000, K. Sato and Y. Iwasa (eds.), Springer-Verlag, Tokyo, pp. 333-338, 2000.

Ataie-Ashtiani, B., S.M. Hassanizadeh, M.A. Celia, M. Oostrom and M.D. White "Effective two-phase flow parameters for heterogeneous porous media," in: Computational Methods in Water Resources, ed. L.R. Bentley et al. (Proceedings of CMWR XIII, Calgary, Canada, June 25-29, 2000), 755-762, 2000.

Ataie-Ashtiani, B., S.M. Hassanizadeh, "Upscaling two-phase flow in porous media with randomly distributed microheterogeneities" in Computational Methods in Water Resources, Eds. S.M. Hassanizadeh, R.J. Schotting, W.G. Gray, and G.F. Pinder Eds. S.M. Hassanizadeh, R.J. Schotting, W.G. Gray, and G.F. Pinder (Proceedings of CMWR2002, Delft, The Netherlands, June 23-28), pp. 1187-1194, 2002.

Ataie-Ashtiani, B., S.M. Hassanizadeh, O. Oung, F.A. Weststrate, A. Bezuijen, 'Numerical simulation of two-phase flow in a geocentrifuge' Computational Methods in Water Resources, Eds. S.M. Hassanizadeh, R.J. Schotting, W.G. Gray, and G.F. Pinder (Proceedings of CMWR2002, Delft, The Netherlands, June 23-28), pp. 225-232, 2002.

Das, D.B., S.M. Hassanizadeh, and B. Ataie-Ashtiani, "Effects of various heterogeneity patterns on capillary pressure-saturation-relative permeability relationships for two-phase flow in porous media, "Computational Methods in Water Resources, S.M. Hassanizadeh, R.J. Schotting, W.G. Gray, and G.F. Pinder (Eds.) Proceedings of CMWR2002, Delft, The Netherlands, June 23-28, pp. 1179-1186, 2002.

Oung, O., A. Bezuijen, B. Ataie Ashtiani, and F. Weststrate, "Transport of two-phase flow in sand: comparison of experimental results of centrifuge tests and numerical simulations", Proceedings of Int. Conf. on Physical Modelling and geotechnics ICPMG'02, Phillips, Guo & Popescu (eds.), Swets & Zeitlinger Lisse, ISBN 90 5809 389 1, St Johns (Canada), pp 355-360, 2002.

Oung, O. and A. Bezuijen, "Development of selective pore pressure transducers and their use to check the validity of 'classical' capillary pressure saturation curves", Proceedings of Int. Conf. on Physical Modelling and Geotechnics ICPMG'02, Phillips, Guo & Popescu (eds.), Swets & Zeitlinger Lisse, ISBN 90 5809 389 1, St Johns (Canada), pp 95-100, 2002.

Manthey, S., S.M. Hassanizadeh, O. Oung, and R. Helmig, Dynamic capillary pressure effects in two-phase flow through heterogeneous porous media, Poroceedings of International Conference on Computational Methods in Water Resources, Chapel Hill, North Carolina USA (June 13 - 17, 2004), Volume 1, pp. 631-644, 2004.

Hassanizadeh, S.M., Continuum Description of Thermodynamic Processes in Porous Media: Fundamentals and Applications in: Modelling coupled Phenomena in Saturated Porous Materials, Eds: J. Kubik, M. Kaczmarek, and I. Murdoch, Institute of Fundamental Technological Research, Polish Academy of Sciences, pp. 179-223, 2004.

Hassanizadeh, S.M., Oung, O., and S. Manthey, Laboratory experiments and simulations on the significance of non-equilibrium effect in the capillary pressure-saturation relationship, in: Unsaturated Soils: Experimental Studies. Proceedings of the International Conference: From Experimental Evidence towards Numerical Modeling of Unsaturated Soils, Weimar, Germany, September 18-19, 2003, Volume 1, Ed. T. Schanz, Springer Verlag, Berlin, pp. 3-14, 2004.

Manthey, Sabine, S. Majid Hassanizadeh, and Rainer Helmig, "Macro-Scale Dynamic Effects in Homogeneous and Heterogeneous Porous Media," in: *Upscaling multiphase flow in porous media: from pore to core and beyond*, Das, D.B. and S.M. Hassanizadeh (Eds.), to be published by Springer, 2005.

- H.K. Dahle, Celia, M.A., and S.M. Hassanizadeh, "Bundle-of-tubes model for calculating dynamic effects in the capillary pressure-saturation relationship,"," in: *Upscaling multiphase flow in porous media: from pore to core and beyond*, Das, D.B. and S.M. Hassanizadeh (Eds.), to be published by Springer, 2005.
- T. Gielen, S.M. Hassanizadeh, H.F. Nordhaug, and A. Leijnse, "Dynamic effects in multiphase flow: a pore-scale network approach" in: *Upscaling multiphase flow in porous media: from pore to core and beyond*, Das, D.B. and S.M. Hassanizadeh (Eds.), to be published by Springer, 2005.

Planned articles (at the time of reporting in 2005)

Berentsen, C.W.J., Hassanizadeh, S.M., Bezuijen, A., and Oung, O., "Experimental evidence of dynamic capillary pressure effect in two-phase flow in a soil sample".

Short scientific introduction.

(Non-authorized translation, please take possible mistakes of the translator into account)

It is generally assumed that the relationship between wetting (w) and non-wetting (nw) fluid phases during two-phase liquid transport through porous media takes place according to the capillary equilibrium relationship

$$P^{nw} - P^{w} = P^{c}_{evenwicht}$$

where $P^c_{evenwicht}$ represents an algebraic function of saturation, s^w . This relation is valid during equilibrium, however under dynamic circumstances it is expected that $p^{nw} - p^w$ will differ from $P^c_{evenwicht}$. Founded on thermodynamic theories the following dynamic relationship was derived:

$$P_{dynamisch}^{c} \equiv P^{nw} - P^{w} = P_{evenwicht}^{c} + \tau \frac{\partial S^{n}}{\partial t}$$

Aim of this project is to find out whether the dynamic effect can be observed under laboratory conditions and whether the new formula describes pressure differences between the two phases more accurately in homogenous and heterogenous porous media. Another research question addresses the relation between $P^c_{evenwicht}$ and s^w for a heterogeneous porous medium on a higher scale. By means of two phase transport column experiments in the geocentrifuge facilities at Delft Technical University, and under normal laboratory conditions, and by numerical model simulations, both questions could be answered satisfactorily. Numerical model results show that the function $\tau(s)$ and the derived $\partial_{\tau} S$ have to be zero for τ =0. Currently the exact form of $\tau(s)$ can not be determined because of the accurateness of experimental results so far. Finally, a two-dimensional numerical model was developed for other research in progress.

Popular abstract.

(Non-authorized translation, please take possible mistakes of the translator into account)

Our soil consists of, among other substances, sand, stone and/or clay particles and granules. Between these particles cavities remain, the pore space of the medium. These pores can be filled with water, air, oil or other fluids. The distribution of the various components (sand, clay, rock, etc.) within a certain volume of soil determines the permeability and porosity. Porosity is the fraction of the medium's volume taken up by pores. Porosity indicates how much fluid a soil can contain. The permeability indicates how easy a fluid can move through a medium. The higher the permeability, the less the resistance/friction the fluid senses, and the easier the fluid can move through the medium. The soil composition differs locally. Characteristics like porosity and permeability depend on the exact location. When a certain volume of soil shows differences in composition within that volume, the soil is called heterogeneous, if the composition doesn't differ within that volume, it's called homogenous. Note that defining heterogeneity and homogeneity depend on scale. Within a square kilometer of land, each square meter can qualify as homogenous, whilst the soil's composition markedly differs between both plot ends.

If we zoom in to individual grains of sand, each pore will prove different, but if a sufficiently large amount of pores is considered together, the fraction the pores make up may turn out to be constant, regardless the number of pores. To an investigator, this invariability is a pleasant characteristic for a soil.

Investigating transport processes in porous media investigates how the different fluids that can be present in soil move through soil. The most simple type of transport is the socalled single-phase transport. In this case the entire pore volume is taken up by a liquid phase (e.g. gas, water or oil). In this case the components of the fluid mix freely. In contrast, multi-phase transport is characterized by several liquid phases being present in the porous medium. The different liquid phases are separated by sharp (clearly visible) phase fronts. In most cases, one of the phases has a "preference" to attach to sand grains. This phase is called the wetting phase. The attracting forces between the sand and the wetting phase are larger than the attraction between the non-wetting phase and the sand. As a consequence, the phase front has the shape of a meniscus, where the pressure in the non-wetting phase at the convex end of the meniscus is higher than the pressure in the concave part of the meniscus (shown in figure 1). The pressure difference between the two phases is called the capillary pressure. A well known example is how water rises inside a straw (Figure 2). When we stick a straw into a glass of water, the water (the wetting phase) creeps upwards along the inside wall of the straw until the downward gravity and the upward capillary pressure match. The capillary rise is higher if the straw is narrower. The same applies to narrower and wide pores.



Figure 1: Capillary interface between water and oil in a pore between 2 grains of sand

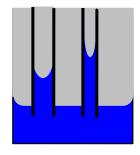


Figure 2: Capillary rise of the water level in a wide and in a narrow air-filled straw

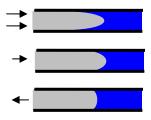


Figure 3: The effect of direction of flow and velocity on the shape of the interface between 2 different liquid phases

From here on we limit ourselves to two-phased flow of water and oil, where water acts as the wetting phase. When two phases flow through a medium, the interface between the two phases is constantly changing shape. The shape of the interface within the pores depends, among other things, on the direction and the rate of flow. The interface will be straighter when water is moving oil, and more convex if oil is moving the water (figure 3). In other words, the capillary difference in pressure between oil and water will be higher when oil replaces water (drainage) the when water replaces oil (imbibition). This effect is known as hysteresis. Besides that, the shape of the interface also depends on the flow rate and the total drop in pressure over the pore. If oil replaces water the interface will become more convex if the oil velocity (or oil pressure) increases.

When modelling liquid transport, it has proven impossible to model the flow behaviour in each pore in the soil individually. Assuming large grains of sands, 0,5 mm in diameter, a square kilometer of a 10 meter thick plot would imply modelling the flow around no less than 10¹³ grains of sand. Besides it being impossible (and not wanted) to gather precise information (shape, surface, stacking, etc) of so many grains of sand, it wouldn't be feasible to model the flow around so many particle within an acceptable time frame by the current stand of computer technology. This problem is circumvented by scaling up smaller models. In stead of modelling the flow within each pre, the soil is subdivided in blocks of a larger volume. If we would subdivide our plot in blocks measuring 5 by 5 by 1 meters, we would 'merely' have to model the flow behaviour within 400.000 blocks. The purpose of upscaling is to describe the essential average flow behaviour on the smaller scale on a larger scale without taking all small-scale details of the smaller scale into account. A problem arises with the definitions. Sometimes, small scale details turn out to be essential for describing large scale flow behaviour. An example would be a porous medium where the flow in the main direction is in part taking place through relatively long and narrow highly permeable pores. The behaviour of a single crack can dominate the flow pattern through the medium. Upscaling is mostly two-tier.

The first step (from pore scale (or micro scale) to macro scale) describes the average flow behaviour of a small homogenous soil sample. On the larger macroscopic scale the pore structure and liquid flow is no longer explicitly modelled. In stead, some unique characteristics are attributed to the soil sample, like porosity, permeability,

saturation, etc. Saturation is the fraction of the pore volume taken up by water. The absolute permeability signifies the ease with which a one phase liquid moves through the soil sample in the presence of a second liquid. This definition is saturation dependent. During this step of the upscaling process it is desirable that the average characteristics per volume are invariant for small changes in sample volume. This means that the behaviour of a single pore may not influence the average behaviour of the soil sample as a whole.

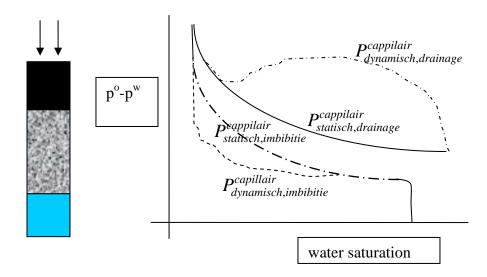
The second tier (from macroscopic to megascopic scale), we try to describe the average behaviour of a volume, regarding the macroscopic scale locally as homogenous. The megascopically upscaled behaviour depends, among other things, on heterogeneities within a block and exchange with the environment.

On the macroscopic scale, water pressure for any block is defined as the volume-average water pressure. The average is only calculated within the volume of water within the block. Similarly, the oil pressure is the average oil pressure within the oil volume within the block. The macroscopic capillary pressure is the difference between the average oil and water pressure.

$$P^{capillair} \equiv P^{olie} - P^{water}$$

During upscaling, so far the capillary pressure was mostly modelled as a function of water saturation alone (or oil saturation alone). Capillary pressure went up with declining saturation with the wetting phase (in our case water). This is directly related to the fact that in a stationary situation capillary forces between two fluids are larger in smaller pores than in wider ones (see figure 2). Whenever oil replaces the wetting water phase, the larger pores are drained first, and more effort is needed to drain water from the narrower pores.

To determine the capillary pressure as a function of water saturation, static or equilibrium experiments are carried out in the laboratory. In such experiments a water-saturated soil sample is placed between an oil reservoir on top (shown in black in the figure below left) and a water reservoir below (shown in blue in the left hand figure below). The pressure from the oil is increased step by step. From a certain oil pressure onwards (the 'entry pressure'), part of the water will be pushed out of the soil sample. After each increment of oil pressure one waits until the flow stops and an equilibrium between capillary pressure and gravity has established. This then results in a single data point in the so-called Pc-S primary drainage equilibrium curve. When, in reverse, the oil pressure is lowered step by, step water from the water reservoir is re-entering the soil sample, and an imbibition curve can be obtained. This equilibrium imbibition curve is always situated below the drainage curve, a direct consequence of the shape of the water-oil-interface on the level of individual pores.



With these static experiments it takes a very long time (several days) for equilibrium to establish. In many realistic situations, the flow conditions tend to change before an equilibrium situation was reached. Laboratory results show that under non-equilibrium conditions it is not justified to regard capillary pressure merely as a function of water saturation. When, for instance, the oil pressure is suddenly increased drastically (in stead of step by step) the capillary pressure curve during drainage (shown in the righthand figure above as " $P^{cappilair}_{dynamisch,drainage}$ " lies well above the statical Pc-S-curve, depicted as " $P^{cappilair}_{statisch,drainage}$ ". On the other hand, during imbibition the non-equilibrium PC-S-curve " $P^{cappillair}_{dynamisch,imbibitie}$ " shows to be situated well below the static imbibition curve " $P^{cappilair}_{dynamisch,imbibitie}$ ".

In recent theory a new relationship between (dynamic) capillary pressure and the equilibrium- or static- capillary pressure was derived. In this relation the difference between both pressures (oil pressure minus water pressure, p°-pw(or p°il-pwater) or p°ile-pwater) is connected to the change in saturation over time:

$$P_{dynamisch}^{capillair} \equiv P^{olie} - P^{water} = P_{statisch}^{capillair} + \tau \left(S^{n}\right) \frac{\partial S^{n}}{\partial t}$$

To obtain an impression of the meaning of the formula above, we'll look at water being replaced by oil (drainage). At a high flow rate, as a result of a high oil pressure, the liquids move fast, and by consequence the change in saturation over time will be large (dSn/dt>0). However, at a high oil pressure the oil/water interface will be more convex than is the case at lower oil pressure, and the (dynamic) capillary pressure will also be bigger than under static conditions. During drainage under dynamic conditions the dynamic Pc-S curve will therefore lie above the Pc-S curve observed under static conditions. With imbibition the story goes the other way round, (dSn/dt<0) and the dynamic Pc-S curve will be below the Pc-S curve observed under static conditions.

Comparing this model to experimental results obtained from homogenous sand samples, shows that this new formula, applied on a macroscopic scale, is indeed capable to describe the dynamic behaviour qualitatively correct. In contrast, the old static equation is not able to explain the 'lift up' of the dynamic Pc-S curve when compared to the static Pc-S curve. It turns out that, in order to reach quantitative agreement between model and experiments, the τ coefficient should be an increasing function of oil saturation, under the condition that both function value τ as well as $d\tau/dS$ have to equal zero. For τ functions that don't meet these requirements, it shows that the initial (sand sample average) saturations is calculated incorrectly. Furthermore, it turns out that the $\tau(S^n)$ coefficient increases with the length scale of the sample under study. For the exact behaviour of $\tau(S^n)$ as a function of oil saturation the model needs to be compared to very precise experimental data.

The effect of (small scale) heterogeneities on the behaviour of $\tau(S)$ is currently subject of research at numerous renowned universities.