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Hydrology and Earth System Sciences Discussions

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Interactive Comment

Interactive comment on "Thermodynamics of the hydraulic head, pressure head, and gravitational head in subsurface hydrology, and principles for their spatial averaging" *by* G. H. de Rooij

G. H. de Rooij

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Reply to anonymous review

Comment 1). As written above, the statement of the upscaling part and the concept followed to define averaged pressures did not become clear to me. This is outlined in more detail below. * It is written in the abstract that consistent upscaling equations are derived for various heads (lines 9-12 on page 1138). To my understanding, upscaled equations would be derived for a problem (a differential equation, including boundary conditions) and not for a variable. The macroscopic variables result from upscaling of a given problem. I think this is often mixed up in the paper.

Response: This comment is in line with the local volume averaging as defined in Quintard and Whitaker (1988) (reference in the paper). I have brought the terminology in line with the volume-averaging literature (and added a discussion of this literature to the Introduction). The upscaled heads are still valid, but I made it clearer that they represent energies stored in volumes of water rather than the energy per quantity of water defined at a point. Thus, they represent well-defined physical quantities of well-defined volumes of subsurface water: potential energies caused by pressure and elevation, as well as the sum of both. They are defined and can be interpreted without having to resort to a particular upscaling method.

I agree with the reviewer that upscaled variables like the hydraulic conductivity and the soil water capacity result from upscaling a given problem. Here I focus on upscaling Darcy’s Law and the hydraulic conductivity, and the definition of the upscaled hydraulic conductivity that I present in the revision indeed arises from upscaling the problem.

To avoid any confusion: it is not my objective to arrive at a full-fledged upscaled flow equation with its accompanying upscaled parameters. From my review of the volume averaging literature I conclude in the revised paper that this requires too many assumptions and limiting conditions to render the upscaled equation practically applicable. I therefore have the less ambitious (but hopefully more realistic) goal of investigating the range of scales for which Darcy’s law can safely be applied.

An alternative way of looking at my approach is from a measurement perspective. Assuming a (hypothetical) set of sensors that record hydraulic and or matric/pressure heads, volumetric water contents, and water flux densities at comparable scales, what would these sensors record, and how would these measured quantities be related to each other as the characteristic length of the measurement volume (heads and water content) or cross-sectional area (flux density) increases? I submit that the volume-averaged heads and water contents, and the area-averaged flux densities measured by well-functioning sensors (without systematic bias and with adequate accuracy) would

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indeed be close to the values computed with the equations presented here. The relationship between them would then be the upscaled Darcy’s Law presented in the paper, which at some point stops behaving in a Darcian fashion, as I hope to have demonstrated.

* The volume averaged porosity and water content and the phase averaged potential is defined by eqns. (8) - (12). It is argued that the phase averaged potential is consistent to thermodynamically defined pressure, as it contains the total energy of the system. In Section 3 the point is made that the vertical coordinate has also to be volume averaged, as any additive term in the potential has to be averaged. Is this not always done this way in "classical" volume averaging theory, if the Darcy equation is averaged (as for example for the macroscopic two-phase problem in M. Quintard and S. Whitaker: Two-phase flow in heterogeneous porous media: The method of large-scale averaging, Transport in Porous Media 3, 357-413, 1988)? The approach in the volume averaging papers is always that the flow or transport equation is averaged, and not the variable. But the gravity term is averaged the same way as the pressure gradient term. A comparison of the definitions given here to the definitions made in volume averaging theory would be useful to clarify this question.

Response: Actually (and luckily) the reviewer is entirely correct here, inasmuch as s/he refers to the classical volume averaging theory. But the one paper that acted as a major stimulus for this work did not, and thus claimed the existence of a ‘paradox’ in saturated flow theory. I demonstrate here that the paradox is non-existent and that the averaging procedure adopted in the first section of that paper is flawed in that it ignores gravity. My line of argument really is that the ‘classics’ (to paraphrase the reviewer) had it right all along. But since the suggestion was made in the literature that they were not, and since I am aware of follow-up work being done in investigating this ‘paradox’ I thought HESS would be a good forum to offer a alternative view.

In the rewritten version there is much more emphasis on the volume-averaging litera-

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ture, and the connection between that body of work and this paper should be considerably clarified.

Incidentally: the solution of the closure problem in the volume averaging literature is in some cases possible only if gravity is ignored.

* It is outlined that it does not make sense to volume average the hydraulic conductivity tensor directly (page 1149, lines 1-3). However, I do not think that volume averaging of the hydraulic conductivity directly would be done in any upscaling approach. I think that all upscaling approaches would proceed from the Darcy equation, average the equation (stochastic average, volume average, or any average) and derive from that an effective conductivity (for example: P. Renard and G. de Marsily, Calculating equivalent permeability: A review, Advances in Water Resources 20, 253-278, 1997).

Response: I know, but since I was developing consistent upscaling formulations I thought it might help to explain why the mathematical consistency in the approach was not extended to the conductivity tensor. Incidentally, in the revised text I follow the approach outlined by the reviewer in inferring the conductivity from the averaged Darcy’s Law, in response to a comment by Dr. Gimmi.

* It is argued that the volume averaged Darcy equation (or flux) does not yield an equation, which has the shape of a Darcy equation, as the potential gradient is coupled to the hydraulic conductivity via the integral. Again: is this not also found in all volume averaging approaches (Whitaker, The method of volume averaging, Kluwer, 1999 for the single phase flow problem and Quintard and Whitaker, 1988 for the two-phase problem)? It is also found in stochastic averaging, only that the integral over the area is there an integral over the ensemble. The problem of the coupling is the same, though. The next step would be to introduce a closure or approximations, which allow to decouple averaged head gradient from the rest and to define this way an effective conductivity. To obtain an effective conductivity that is independent on other variables or boundary conditions is only possible for simple conditions, for example, if boundaries

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are far away from the region of interest. For simple conditions it has, however, been demonstrated very often that the effective conductivity is approximately independent of the averaged pressure head (for example, P. King, The use of field theoretic methods for the study of flow in a heterogeneous porous medium, Physica A, 3935 - 3947, 1987).

Response: The key phrase in this comment is ‘For simple conditions’. The voluminous literature on the closure problem in variably invokes numerous simplifications, most notably the clear hierarchy of scales, with the pore-scale, the scale over which volume averaging takes place, and the scale for which large-scale averaged quantities can be derived being well separated. Quite often, the degree of mobility of phase interfaces is restricted, limiting the applicability for three-phase systems to quasi-steady flows. The local values within an averaging volume of any quantity that needs to be volume-averaged are generally described as zero-averaged deviations from the large scale intrinsic phase average. Certain restrictions may apply to the magnitude of these deviations. The development that I present here only requires that Darcy’s Law is valid at some scale (paramount to requiring that a representative elementary volume exists), and that energy and mass are conserved. The main motivation is that in many problems, particularly in unsaturated soils but also in aquifers, the scale of the problems to be solved often is too small to meet the requirement that its scale is much larger than the volume-averaging scale. Furthermore, natural porous media often exhibit heterogeneities at any scale of observation (pore size variability, layering and spatial trends within layers, lenses of contrasting grain sizes embedded in sediment strata, etc.). I therefore do not believe the required separation within the scale hierarchy always exists. These concerns do not invalidate the volume-averaging literature, but the do provide justification for a more generally applicable study that necessarily must lose some of the mathematical sophistication that relies on the above restrictions.

In the revision, I have adapted the treatment of the effective hydraulic conductivity in a way that allows an examination of the conditions under which it acquires properties for which Darcy’s Law can be used with confidence.

* At the end of Section 2.2 the statement is made that the total energy concept does not hold for macroscopic pressure, as the phase averaged potential does not appear in the areal averaged Darcy equation (page 1150, lines 21-22). I cannot follow this argument. If for some reason one decides that the macroscopic variable of the problem has to be the phase averaged potential: why is it not possible to try to write the equation in a way (for example by multiplying and dividing by the water content) that the phase averaged pressure would be the macroscopic variable? It is very likely that the resulting problem would be a mess, and it will not look like a Darcy equation for sure, but I do not think that it is in principle impossible to derive an upscaled problem, which has the phase averaged pressure as macroscopic variable.

Response: The actual text of the original manuscript reads:’…the total energy of a body of water is of little use in describing its tendency to generate subsurface flow.’ This statement simply reflects the conclusion that there is no clean upscaled version of Darcy’s Law that produces areally averaged flux densities across an arbitrary plane from the areally averaged gradient of the hydraulic head across that plane. Please note there was a weighted phase average of the potential gradient in the upscaled formulation of Darcy’s Law, and in the new formulation presented in the revision there still is. Therefore, in my view, the statement attributed to me in a paraphrased form by the reviewer is not supported by the text as I wrote it. As a consequence I am not quite sure how to incorporate this comment. Nonetheless, in the remainder of the comment the suggestion is made to develop Darcy’s Law in terms of a phase-averaged pressure. Apart for my preference to us the averaged potential rather than the pressure to include the effect of both pressure and the position in the gravity field, I believe I have done so in the updated version. Although the upscaled version of Darcy’s Law lacks the elegant simplicity of the original local version, I hope the reviewer will agree with me that rather than being ‘a

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mess’, it has a form from which much can be learned by careful analysis of its various terms.

Comment 2). In Section 3 the phase average is applied to derive an averaged retention function. What is the explanation that this the most consistent or reasonable way to average the retention function? It would be the definition, which is consistent to the total energy concept. But would it not depend on the measurement device or the problem one is interested in, how the upscaled retention curve should be defined?

Response: That depends on the flexibility one allows itself in defining the conditions that are allowed. In the laboratory, the water retention curve is determined under equilibrium conditions on a small, and preferably relatively flat sample. Since I was interested in larger scales I only maintained the equilibrium requirement, and I developed an expression between volume-averaged water content and matric head for an arbitrary volume. The shape and size of that volume may very well depend on the instrument used and the intended application.

This comment made me realize one could also opt to design an experiment or conditions in which the matric head would be uniform throughout. That would necessarily result in unit gradient flow, in which the imposed downward flow could be varied to arrive at different matric heads. Or, in case of naturally occurring conditions as in areas with deep groundwater tables, where unit gradient conditions prevail at some depth below the soil surface, one could observe matric heads and water contents to arrive at data points on a steady-state rather than an equilibrium water retention curve. (Of course, under natural conditions one can only cover a limited range of the large-scale water retention curve, and possibly obtain only a single data point.) For this condition, expressions for the volume-averaged water content and the various head arise naturally, and the paper was adapted accordingly.

Comment 3). I do not understand eq. (14). If K_j,A is really the areally averaged hydraulic conductivity, the answer to whether an averaged gradient could be found that

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enforces eq. (14), I think, is no. The non-averaged Darcy equation cannot be brought into the shape of eq. (14) with any weighting function without dropping terms. Should not the question rather be if an equivalent hydraulic conductivity (K_eff, not K_A) can be found, so that under reasonable approximations, the averaged Darcy equation could have the shape of a Darcy equation?

Response: This part of the text was rewritten in response to other comments. The new text addresses the final remark of this comment.

Comment 4). Why is it is meaningless to volume average flux (page 2249, lines 4-5)? A volume average can be considered as a filter, and I do not find it inconsistent to filter the flux field. It might be that it is not a measurable quantity and to compare to measurements an average over the plane might be more appropriate. But in general I do not see what is wrong with volume averaging flux. In the paper a reference to the paper of Nordbotten is given, but an explanation would be helpful.

Response: An interesting comment that puzzled me a bit. Earlier, the reviewer explained it was obvious that the conductivity would never be averaged directly in any upscaling approach, yet here s/he wonders why the flux density should not be volume-averaged. But the conductivity is simply the flux density for unit hydraulic head gradient, and thus these comments seem contradictory. A brief explanation as to why volume-averaging flux densities are of little value: in deriving differential equations for flow, the fluxes across the boundary of the elementary volume appear in the mass balance. As we move to larger scales, the fluxes over the boundary of the larger volume appear; internal fluxes cancel out in the mass balance. To conserve mass at the larger scale, the normal component of the flux density over the boundary of the volume of interest is integrated over the boundary (amounting to the application of Green’s theorem). This is well-established (see for instance Raats and Klute, 1968a [full reference in the paper], and I am a bit reluctant to put in the paper to avoid stating the obvious.

The comment seems to reflect a change in approach over the years. In the early

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literature (1960’s, 1970’s) the method of choice for large-scale problems was to work with integral equations rather than differential equations and invoke Green’s theorem to work out the mass balance of the volume of interest (I am indebted to Pieter A.C. Raats for this reply). In the later volume-averaging literature, fluxes across boundaries were frequently approximated by some volume-averaged flux density, but this is obviously an approximation that can only be exact for limited conditions. Since I did not endeavor to solve any closure problems, I preferred the more exact approach in order to limit the necessary assumptions.

The reviewer’s view of the volume average as a filter sheds some light, and merits attention, particularly in conjunction with Quintard and Whitaker (1988), referred to above by the reviewer, and denoted QW from here on. Equation 1.14 in QW gives a volume-averaged velocity in an exact analogy to the volume-averages defined in the paper here. The gradient of this volume-averaged velocity is then used in Eqs. 1.11 and 1.13 in QW to establish the mass balance of two fluids at the point-scale in a locally averaged medium in which the pore-scale intricacies have been averaged to allow a continuum formulation. This velocity gradient approximates the differences between ingoing and outgoing fluxes at opposite sides of a cubic elementary volume, which can be exactly defined in terms by a surface integral over the entire surface of the cube of the normal components of the velocity vector. The approximation holds because of the provision explicitly stated by QW that the length scale of the averaging volume is much smaller than the characteristic length scale associated with local volume-averaged quantities. Under this restriction, the volume-averaged can indeed be used as a filter (in the reviewer’s words), but I make no such provision. Therefore, the equations I developed have more generality at the cost of having to disallow volume-averaging.

Comment 5). The sentence on page 1150, lines 18-21 is somewhat confusing. The coupling of the head and the conductivity for the averaged problem generates a non-linearity, but the Richards equation is non-linear in its non-averaged form and not only

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due to coupling of head gradient and conductivity.

Response: The sentence meant to convey that in Richards’ equation, the hydraulic conductivity is a function of the matric head whereas, in saturated flow, the (saturated) hydraulic conductivity does not depend on the hydraulic head. But in the upscaled version of Darcy’s Law, even under saturated conditions, the hydraulic conductivity is a function of the hydraulic head, making it more similar in that respect to Richards’ equation. This part of the text was removed in the revision.

Final response: Overall, the two reviewers provided valuable and constructive comments, but suggested diametrically opposed revisions. In view of the reviewers’ opinions, and those of others that were received by me but not committed to the HESSD website, and after informal discussions with various colleagues I decided to remove the thermodynamically oriented section of the paper and focus on the upscaling, thereby refocusing that part in response to the more critical comments of the anonymous reviewer.

Interactive comment on Hydrol. Earth Syst. Sci. Discuss., 5, 1137, 2008.

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