

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

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The manuscript by G. H. de Rooij deals with the upscaling of variables and equations that are typically used to describe water flow in subsurface hydrology from a small REV scale, at which elementary properties of the soil considered as a continuum are defined or measured, to larger scales, which are typically relevant for problems of interest. I think that this is a very relevant topic and especially interesting from a fundamental point of view, even though the 'real-world' consequences may be minor in many (but not all!) cases.

The manuscript is well written and I enjoyed reading it. In fact, I think that the author

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succeeded well to summarize complicated matter in a clear manner. I have, though, the feeling that it needs a careful revision because of two reasons. First, I consider some of the arguments presented in the development of the upscaled equations as not fully convincing (see comment 4 below). Second, at several places it was not fully clear to me, what exactly is new or different compared to earlier work, and what is just reported from earlier work (see comment 3 below). In this context, I had the impression that the type of paper is not clearly defined: review or research paper? (See also comments 1 and 2).

Main Points

1) Does the title reflect the contents of the paper?

I have the feeling that the title emphasizes too much the first part (thermodynamics of the hydraulic head, pressure head, and gravitational head). It is not so clear to me, to which degree Section 2.1 just summarizes existing work, and to which degree it really introduces new or different concepts (see comment 3 below). I feel that the manuscript is more focusing on the upscaling of the water retention curve and the Darcy equation, and not so much on the thermodynamics of the hydraulic head. Accordingly, I suggest to adapt the title (but see also comment 3).

2) Aims of the paper

I am a bit confused about the main focus of the manuscript. In the abstract, it is stated that 'a thermodynamic justification of the theoretical relationship between the hydraulic, pressure/matric, and gravitational head' should be given, as well as 'consistent upscaling equations for the various heads'. Later, in Section 2.1, I have the feeling that the manuscript presents mostly a (nice and helpful) review or a summary of existing literature, but it is not clear to me which equations give the intended 'thermodynamic justification' (see also comment 3). Section 2.2 deals with upscaling, but mostly upscaling of the Darcy equation, which was not mentioned in the abstract. I think that the author should clarify the aims of this paper in the abstract (or change the text of 2.1,

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see comment 3). In the introduction (especially at the end), the aims are more clearly declared, even though I feel that there as well the author could be more specific (e.g., which soil physical variables are considered?).

3) Aim of Section 2.1, new aspects

This Section seems to be mainly a review – at least it is difficult for me (not being familiar in detail with all the cited references) to find out, in which respect the equations given here differ from earlier work. It is perfectly ok, of course, to present a review on existing work, especially if this information is required later. However, I think the paper would benefit if either the new aspects in this Section would be presented more prominently, or the expectations of the reader would be channeled in a different direction by clarifying the focus in the Abstract and Introduction (see also comments 1 and 2).

4) Derivation and significance of Eq. (16), Section 2.2

Eq. (13) shows the average $q_{j,A}$. Using a weighting function of 1 for q (according to the middle term) seems justified, because q refers to the total (local) cross sectional area, i.e., the local q are uniformly distributed over the area A (weighting with the local θ is already implicitly included).

According to Eq. (14), the average $K_{j,A}$ is obtained as $q_{j,A} / (dH/dx_j)_A$, where $(dH/dx_j)_A$ is the average gradient of H that is calculated with the unknown weighting function f . Then, the author states that he doesn't consider θ as a reasonable weighting function and assumes (arbitrarily) $f=1$. With this assumption, he obtains the result of Eq. (16), which shows that an average $K_{j,A}$ can be obtained from the average $q_{j,A}$ and the average gradient calculated with $f=1$, and that this $K_{j,A}$ represent then an average of the local K_j weighted by the local dH/dx_j .

This is correct, in my opinion, but not a unique solution. In fact, instead of $f=1$, any other weighting function could be used in Eq. (14), and accordingly a different average $K_{j,A}$ would be obtained. Let us denote the weighting function to obtain $K_{j,A}$ as g . In

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general, we have two unknowns, either $K_{j,A}$ and $(dH/dx_j)_A$, or g and f . A solution for one of the two unknowns has little physical significance, unless an independent determination of f or g , or $K_{j,A}$ or $(dH/dx_j)_A$, is possible.

So, because f was arbitrarily set to 1, I consider the statement on p. 1150 l. 12f, "... that the areal average of the flux density involves arithmetic averaging of the gradient of H " as incorrect, or at least not as a general result. Similarly, I think the statement on the same page, l. 7ff ("According to ... hydraulic conductivity of A is found by weighting the local values of K_j by the local hydraulic head gradient...") is not general either. The average $K_{j,A}$ presented is just one possible expression, which is obtained by setting $f=1$. Accordingly, I don't think that the derivation presented proves that "upscaling Darcy's Law through consistent averaging of H and K while keeping the differential equation itself identical to its point-scale form .. is impossible". This may indeed be the case, but it is not proven here in my opinion.

I think the author should make this clear in the text. Without a good justification why f should be equal to 1, the result bears little significance.

Just in parentheses: I can think of another way of proving that a consistent upscaling of the Darcy equation may lead to a different differential form – but this is more an idea and may also not be rigorous. I denote an average with $\langle \rangle$. When upscaling the local Darcy equation, $q_j = -K_j dH/dx_j$, we have

$$\langle q_j \rangle = - \langle K_j dH/dx_j \rangle,$$

which can be evaluated as

$$\langle q_j \rangle = - \langle K_j \rangle \langle dH/dx_j \rangle - \text{Cov}(K_j, dH/dx_j),$$

where Cov means the covariance. This equation shows two things: First, there is an additional term in $\langle q_j \rangle$ compared to q_j , the covariance, which disappears only when the local K_j and dH/dx_j are uncorrelated. At the local scale, it seems unlikely that K_j depends on dH/dx_j , but dH/dx_j will likely depend on K_j (and even the

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neighboring K) in a heterogeneous system, so this covariance term does probably not disappear. I think that this becomes especially evident when considering the development of anisotropy: locally isotropic media can give rise to an anisotropy at the larger scale. Second, the average $\langle q_j \rangle$ depends on $\langle dH/dx_j \rangle$, and not on $d\langle H \rangle/dx_j$, as would be required for a consistent upscaling of the primary variables of the Darcy equation. In general, $\langle dH/dx_j \rangle$ is not equal to $d\langle H \rangle/dx_j$, because $\langle dH/dx_j \rangle = \text{Integ_A}[f_{(dH/dx_j)} dH/dx_j dA]$, where $f_{(dH/dx_j)}$ is the pdf for dH/dx_j , and $d\langle H \rangle/dx_j = d/dx_j\{\text{Integ_A}[f_H H dA]\}$, where f_H is the pdf of H . Unless $f_{(dH/dx_j)} = f_H$, the two averages are not the same.

5) Example of macroscopic flow, Section 3.2

I think this section is really, as the author states at the beginning, just a generalization of the work of Gray and Miller (2004). At some places in the manuscript (e.g., p. 1138 l. 13ff; p. 1141 l. 22ff; p. 1154 l. 1ff), it sounds as if the work here was a correction of the work of Gray and Miller (2004). This is not correct, in my opinion; Gray and Miller already made clear in their paper that neglecting the gravitational potential in the upscaled horizontal flow problem leads to incorrect results; the "erroneous" derivation had just illustrative character. So I think it is not correct to state that "an apparent paradox reported in the literature" is resolved, as done on p. 1138 at the end of the Abstract.

Minor Points

6) Details given when referencing to other work

I think that the Introduction and Sections 2.1 and 2.2 give a good overview. In some cases, though, I feel that the author should give some more information, otherwise it is sometimes difficult to follow the text. Examples: p. 1139, work of Nordbotten et al. (2007); p. 1140 l. 20: Unclear: Sounds as if the averaging makes the fractions hysteretic; p. 1143 l. 19ff: In which sense are the pressures ambiguous in Gray (2002)?

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7) Scales considered

I think that the definition of the scales that are considered in this paper is very important. The author introduces the definitions for the REV scale or the Darcy scale on p. 1138f, but later he uses also the term macroscale (e.g., p. 1140 l. 4; p. 1144 l.7ff). I suggest that this term is also introduced at the beginning.

Details

- p. 1141 l. 7 and 22: "They reported inconsistencies...", I think one should write something like "They reported apparent inconsistencies..." (see comment 5)
- p. 1143 l.21: I would cancel "unit gradient or"
- p. 1144 l. 16: "than" instead of "then"
- p. 1146 l. 10: I would change the title of Section 2.2 for instance to "Upscaling from the Darcy to larger scales by spatial averages" to define clearly the range of scales considered
- p. 1148 l. 5: delete "and"
- p. 1148 l. 9: I would continue with "The latter identifies... " instead of "which..."

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