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Interactive comment

Interactive comment on "On the Consistency of Scale Among Experiments, Theory, and Simulation" *by* J. McClure et al.

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Response to Review #1 of
On the Consistency of Scale Among Experiments, Theory, and Simulation
J.E. McClure, A.L. Dye, W. G. Gray, and C. T. Miller

1 General

We respond to the comments from Referee #1 beneath comments made. The authors' response is shown in red.

2 Referee #1

The paper critiques current models and makes a case for developing models that are consistent across scales based on thermodynamic principles. The nature of the processes these models tackle is kept vague, but some hints suggest that models for subsurface water flow (soil water and groundwater) are the prime target. A theoretical treatment of the Laplace Law is developed to develop equations for microscale capillary pressures, which seems to refer to pressure jumps across fluid-fluid interfaces in single pores. These expressions are more general that the Laplace Law because they apply to equilibrium and non-equilibrium cases. Expressions for average intrinsic phase pressures are also presented.

An experiment is described in which a non-wetting gas phase (nitrogen gas) permeates a 0.5 by 0.5 mm two-dimensional porous medium saturated by a wetting fluid phase (decane). This process and similar ones with different initial and boundary conditions are also modeled numerically. Both the simulated and observed data are used to obtain the 3D equivalent of the decane retention function in which the degree of saturation is a function of both the average fluid pressure and the specific interface area.

Major comments

For a paper on scales I could not help noticing that the time scale is mentioned only once and that there is no clear definition of the spatial scales of interest (microscale and macroscale). No connection is established between these scales and the scale of the representative elementary volume.

AU: The time scale does not affect the form of the equations relied upon in this work. In fact, this work is primarily concerned with equilibrium states, how to best explore the potential states that can exist, and how the state function of capillary pressure can be represented. The reviewer is mistaken that the microscale and macroscale are not connected, as all of the macroscale quantities defined and used in this work are defined completely and explicitly in terms of microscale quantities—thus making the connection that the review claims is missing. We could add explicit definitions of the microscale and the macroscale terminology that we use in this manuscript, and incorporate additional discussion on the scale required to obtain a representative elementary volume.

The paper uses a few straw man arguments. It is claimed that in experiments, pressures are only measured (or set) at the boundary of the system of interest. With the increased use of microtensiometers this is no longer necessarily the case. In my experience (and with some support in the literature), the microtensiometers tend to confirm that the known pressure at a boundary can be used to calculate the pressure anywhere in the system as long as contact is good and equilibrium has been achieved. The reliance on boundary pressures is not as risky as the authors appear to believe. In the terminology of the analysis of the paper this implies that phase continuity in real-world porous media is often sufficient for the observed pressures to be valid.

AU: We agree with the reviewer that microtensiometers provide a means to measure fluid pressures within a domain, and we can note this in a revised manuscript. We also agree with the reviewer that if both fluids are well connected across an experimental cell and at true equilibrium state, the boundary condition measurements and microtensiometer observations should be in agreement. We

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disagree with the reviewer that such observations are adequate for characterizing the state of a porous medium system in a general sense, and the results presented in this manuscript clearly support our view. For example, imbibition is well-known to result in disconnected non-wetting phase regions, which will not be connected to the boundaries; the formation of disconnected pendular rings of wetting phase is also well-known. Only if sufficient observations of the pressures of each of the disconnected regions and their morphological characteristics were available would the state of the system be adequately characterized.

This does not mean that the associated capillary pressures are inaccessible from experiment. On the contrary, the increased use of x-ray micro-computed tomography (μCT) makes it possible to directly measure the interfacial curvature within 3D experimental systems. This approach has been used for about 20 years and is now used routinely (e.g., ; ;). As stressed in the manuscript, the true capillary pressure is the product of the average curvature and the interfacial tension. The average curvature can be determined directly from experimental μCT.

The authors state that average phase pressures are convenient to work with. I have never read anything in support of this argument. There are no sensors to measure average pressures, so we cannot calibrate models on them, and I have not come across any work that used average pressures in lieu of local pressures and pressure gradients.

AU: Several measures of pressures are important and come directly out of the TCAT theory. These include volume-averaged pressures, interface-averaged pressures, and pressure averaged over a boundary of a system, such as is the case with conventional pressure-saturation experiments. Common existing measurement methods provide averaged quantities due to the size of the instrument. Mechanistic conservation of momentum models include volume-averaged pressures, so from this perspective such quantities are convenient to deal with. Models are developed based on equations that use average pressures and thus must be calibrated and validated in terms of average pressures. It is precisely the dis-

tinctions among the different measures of pressures that are a key aspect of the phenomena explored in this work. For theory, models, and data to be mutually useful, they must have a common usage and understanding of pressure. We can highlight these points in a revision of this work.

I have the impression that the analysis is valid for zero-gravity conditions. This is never stated explicitly, but three elements of the paper suggest it:

- the casual averaging of pressures without acknowledging the immense effect of the geometry of real-world fluid bodies on the average pressure when gravity is non-zero?
- the implicit notion that fluid interfaces and common curves have a non-zero thickness and therefore mass, without the effect of this mass being discussed or even mentioned.
- the extremely small size of the porous medium used in the experiment that indeed makes the effect of gravity negligible. In a paper in which the introduction discusses the importance of consistency of scales for scale ranges that are many orders of magnitude larger and already in the abstract calls for models that are based on rigorous multiscale principles this severely limits the relevance of the paper.

AU: The TCAT theory relied upon in this work includes the effects of gravity in large systems and for interfaces that contain mass; references to this theory are provided. In this work, gravitational effects were considered to be negligible due to the size of the system, which we will be sure is clearly noted in a revised version.

The lack or relevance is further reduced by the experimental scale: 0.25 square millimeter is in the sub-Darcian scale for most soils and geologic materials. To call this scale the macroscale seems to betray a fundamental lack of understanding of the concepts of the continuum approach and the representative elementary volume that form the basis that most currently used models are founded on.

AU: The reviewer is mistaken. The actual physical size of a system is not an appropriate measure of whether a system is an REV or not. Karst systems may require 100's of meters for a valid REV, whereas microfluidic systems of the sort relied upon in this work can satisfy the physical and mathematical requirements for an REV at length scales on the order of 500 μm or less quite easily. At the microscale, the laws of continuum mechanics apply for a fluid at length scales that are long compared to the mean free path between molecular collisions. For the particular system investigated, the continuum limit would be easily satisfied with a length scale of 1 μm. A valid macroscale requires a clear separation of length scales with the microscale and the resolution scale needed to characterize the pore morphology and topology. This scale usually translates to systems with a length of at least 10 mean grain diameters on a side. While the systems investigated are physically small, they are close to an REV in size. The actual physical size cannot be examined in isolation in reaching conclusions about whether a system is an REV. The systems investigated in this study were sufficiently large to show the occurrence of many regions of disconnected phases, which was sufficient to investigate the state function for capillary pressure. We would add some minor discussion about the size of an REV for porous medium systems and reference these comments to the literature.

Section 4 “Approach” has a non-informative title. It can easily be split in a “Theory” section (modify the title as desired) and a “Materials and Methods“ section, thereby making the paper conform to the established structure of scientific papers. The Results and Discussion section is already there.

AU: This appears to be a matter of style preference. Information in the text and cited references provide sufficient background such that experiments used in

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this work could be reproduced. We note that the HESS guidelines for manuscript preparation do not explicitly require a "Materials and Methods" section. Our manuscript conforms to the structure established in the HESS guidelines. For a serious reviewer to imply that a paper that does not use his or her preferred section headings violates the "established structure of scientific papers" is astonishing.

Section 4 starts with a treatment of the Laplace Law. One of the authors published an extensive treatment of this law (Hassanizadeh and Gray, 1993, not quoted in the paper). I would like to see included in this paper an explanation of the added value of the current discussion in view of this earlier work, and how this treatment relates to that in the earlier work. There are marked distinctions in notation between the earlier and the current paper which made it hard for me to establish the relation.

AU: A quick search on Google for "capillary pressure porous media" provides over 1M hits. A similar search in Google Scholar provides almost 0.25M hits. We can hazard a guess, with confidence, that many of these papers have made useful contributions to the study of porous media. It is clear that the authors have not seen fit to cite much of this wealth of information. Even the authors of this paper have been engaged in a good number of papers that deal with porous media physics and capillary pressure. We have chosen not to cite most of these as well because they are tangential to the mission of the current paper. We can say, with confidence, that our work through the years has demonstrated a development in theory and understanding. We have not been stagnant and insisted on sticking with theories and understandings that have become dated or outmoded. Indeed, reports on developments of new theories, experimental tools, experimental techniques, and simulation algorithms do not necessarily provide reports on or references to older methods that the current work supersedes. For the case at hand, the reviewer seems to admire the 1993 paper, and we appreciate that. This 23 year old paper made a contribution at

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that time. The discussion of the microscale capillary pressure is informative. Frankly, the discussion of the macrocale capillary pressure has been surpassed by understandings gleaned from careful development and application of the TCAT method. This does not negate the contribution of the older paper; neither would a comparable statement about any of the 0.25M citations dealing with capillary pressure in porous media negate their contributions. We can suggest that the reviewer might benefit from looking at more recent contributions in this area of study. We believe that citing one's own work can be self-serving when that work is dated and not particularly pertinent to the issue or issues under discussion in a newer work. We prefer to include references that best serve the hydrologic community that seeks to understand what we are working on and the nature of our contributions. For this reason, we do not cite the 23 year old paper; neither do we provide an extensive review of developments in understanding of capillary pressure, particularly at the macroscale, over the same period. We have a focused set of objectives we wish to address in this manuscript; we employ theoretical, experimental, and computational approaches for doing so. We cite references that are helpful and/or fundamental to fulfilling the objectives of our paper. We see no technically sound reason to cite the paper the reviewer refers to.

The notation used here is explained carefully, and references are given to other works where this notation is explained in detail and used for a variety of applications. Indeed, even when a work involves a more advanced and precise notation than previously used, authors do not have a responsibility to explain and account for the myriad of notations that are used in the same field or in earlier incarnations of work.

The work culminates in a relationship between capillary pressure, degree of saturation, and specific interfacial area. As long as the latter cannot be measured on 3D samples, the work has no chance of becoming applicable.

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AU: We disagree with the reviewer, who seems to be unaware of the considerable amount of active research in this area. Specific interfacial areas are indeed routinely measured in 3D samples now. We present simulations in this work where those quantities are evolved and compare virtually identically with experimental observations. Fast imaging methods are now capable of measuring specific interfacial areas dynamically and nondestructively. The state equation for capillary pressure depends upon a sufficient set of measures of the morphology and topology of the pore space, along with fluid and solid properties. There is no question that specific interfacial area is one of these quantities, as has been well established in the literature. We would like to add that the functional dependence we propose is correct. In itself, that is important. In practice, one does not discard a correct theory in favor of an incorrect one simply because quantities in the correct theory may be difficult to measure. In the present case, the theory is correct, and the results of the combined theoretical, experimental, and computational studies in this paper are moving the theory forward to becoming applied and employed.

I do not see a path for using this kind of work to arrive at the thermodynamically consistent, scalable models for porous media found in nature, even though the authors claim that goal to be a main motivation for the paper.

AU: The reviewer may not see the path; but it clearly exists. We have cleared most of the brush obstructing it. Many visionary researchers are making progress in obtaining appropriate scalable models for porous media. We can caution that some researchers have claimed to have a model that is "thermodynamically consistent" that, in fact, is not. The work here provides a different and correct direction. In general, we do not think that determinations on whether research should be conducted or presented should be based on the suspicion of one individual (or a few or even many individuals) who claims to have limited vision. The reviewer provides no concrete comments based upon scientific

observations but only identifies his/her lack of vision and chooses only to speculate idly. No changes will be made in regard to this speculation.

Overall assessment

The paper has six objectives that claim to resolve several issues relating to capillary pressure at the micro- and the macroscale and expose limitations of conventional approaches.

The Introduction and its list of objectives raise high expectations about the impact and relevance of this paper for modeling of multiphase flows in soils, aquifers, oil deposits, etc. These expectations are in no way met, either by the theoretical analysis that adds only incrementally to an earlier paper and omits gravity, or by the experiment on 0.25 square mm of an artificial, two-dimensional porous medium with two fluids that have no relevance for hydrology. To make the contrast between this work and real-world hydrology even more glaring, the authors drop the name of Eric Wood, who has worked on continental and global hydrology.

AU: We disagree with the reviewer. On page three we list six objectives, each of which is clearly addressed in the material that follows. Because this manuscript was submitted to be part of a special issue in honor of Professor Wood, it seems appropriate to link this work with the work of Professor Wood. His work and this manuscript deal with issues of scale in hydrologic systems. We believe the treatment and tribute is appropriate. We can add that the theoretical approach that is employed here for small systems can be and has been employed for larger systems. The overriding common thread is “change of scale." The tools for achieving this are the same, the applications are different.

The presentation of the material is messy:

- the Introduction dwells on subjects not at all covered by the paper and fails to

inform the reader about the paper's focus and nature of the work.
AU: The Introduction purposely links issues of interest to a broader community to the issue of scale as important for porous medium systems. The present form seems appropriate given the nature of the special issue.

- the list of objectives is too long, and vastly overstates what the paper actually delivers.
AU: The list of objectives is short and each objective is accomplished in the text that follows. It is not clear what the reviewer finds to be overstated or undelivered.

- the paper is not well structured - there is no Materials and Methods section, and the flow of thought is sometimes hard to follow. Some parts are well written, others much less so. A strict adherence to the established format of a scientific paper would help.
AU: We have adhered to the format established by the guidelines for manuscript preparation that are available from HESS online.

- not all variables and symbols are explained, and there are inconsistencies in the notation
AU: This comment is again made without evidence. What inconsistencies? What isn't defined? We have attempted to ensure that each variable is defined. If we have missed any or some, we regret that and would be delighted to address that oversight. We will double check the notation. The reviewer could provide a service by identifying any issues he/she has discovered.

- the description of the experiment and the computations (what should be the Materials and Methods section) is incomplete.
AU: An experimental methods section could be added, although the methods are standard and have been previously published. We don't believe these additions are necessary, and think they would distract from the thrust

of the paper and unnecessarily lengthen it. References to experiments and computations are provided. The reviewer seems to be hung up on some preconceived notion of the organization of a scientific contribution that seems to overwhelm his/her ability to assess the actual contents of the contribution. We prefer not to add more details on the experiments and computations as this would be redundant and would add unnecessary clutter to the literature. We will respond to the editor's request.

AU: The authors will be happy to go through the manuscript and consider changes that might be appropriate in light of the review comments and our own view of the work. We note that this reviewer made a number of detailed and useful comments in an attached document, and we welcome the opportunity to consider incorporating this information in a revision of this manuscript.

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