Interactive comment on “Dynamical process upscaling for deriving catchment scale state variables and constitutive relations for meso-scale process models” by E. Zehe et al.

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First of all we want to thank Keith Beven for the critical but constructive points addressed in his review. The following lines will explain how we addressed his comments in the revised manuscript or, if we didn’t, why we didn’t.

Keith Beven: I have actually commented on an earlier version of this paper (and that of Lee et al.) before it was submitted, and have also included some comments in my paper for the same special issue. However, although I appreciate that I saw and commented on the paper only shortly before it was to be submitted, I did expect to see at least some response to my comments in the submitted version (even if only to include some of the citations I suggested). It is therefore somewhat disappointing to
find that this is not the case. Response: Time was really too short to pick up those comments, as we were already much behind the deadline.

Keith Beven: I think the approach to implementing the REW concepts taken in this paper is a real missed opportunity. I also think that it is unacceptable to just ignoring past work that is contradictory to the assumptions made in this paper approach (e.g. Binley et al., WRR 1989 study of whether effective parameters work at larger scales). Neglecting to mention past studies of using detailed modelling to find functional forms at larger scales (for example, the UP model of Ewen et al. HESS 1997; or the Topkapi model, e.g. Liu and Todini, HESS,2002) is also unfortunate.

Response: In the new approach we refer to the work of these authors. In the old and of course the new manuscript we referred to work of Attinger 2003, Lunati et al., 2002 and Vogel and Roth, 2003 are, from our point of view, of similar relevance in this context.

Keith Beven: After all the appeal to physics on which the REW concepts are based, it seems singularly perverse to then neglect the physics when choosing a representation at larger scales. The fact is that simple physical reasoning suggests that using local scale equations with average or effective parameters to include the effects of heterogeneity and macropores do not work - this was demonstrated more than 15 years ago and it has not been established that it will work in this paper. The main idea of the REA work (that representing the heterogeneity as a distribution of responses might still be important at larger scales even if the pattern is not) also seems to have also got forgotten.

Response: We are not sure, what Keith means with ignoring physics! We definitely do not take point scale equations with averaged of effective parameters as claimed by Keith Beven. What we do is proposing a process model based framework for deriving constitutive relations: a capillary pressure - saturation relation and a relation of hydraulic conductivity as a function of u-zone saturation at the REW scale. Hence we employ a model to derive this relation which is than used with the REW scale mass
balance equations! Keith mentions the study of Binley et al. (1989). The authors employed a full three dimensional model based on Richards-equation coupled with a simple linear routing approach for deriving hillslope scale effective hydraulic conductivities for stochastically generated heterogeneous parameter fields. It is quite interesting that this worked well for weakly heterogeneous systems of high average hydraulic conductivities ranging for 0.05 to 0.2 cm/min (compare their Table 2). They didn’t succeed in obtaining effective hydraulic conductivities that yielded good results for subsurface and surface flow at the same time in case of systems of low average permeability (see their Table 3). The Weiherbach catchment is composed of weakly heterogeneous hillslopes, as described in Zehe and Blöschl, WRR 2004; Zehe et al. 2001 Physics and Chemistry of the Earth. This is strongly supported by the fact that model structures, that just represent the deterministic patterns of soils at the hillslope scale (and neglect small scale heterogeneity) are sufficient to yield model results that match tracer observations at the hillslope scale and rainfall runoff at the catchment scale! The statement of Keith, that our approach cannot work is somehow contradicting to what Binley et al. (WRR 1989) presented in their paper!!

In detail we focus on the exchange processes between the unsaturated and the saturated zone, which can either be capillary rise (i.e. we need a capillary pressure-saturation relation) or recharge! As we still cannot measure average recharge and capillary rise at that scale, i.e. by hillslope scale drainage and wetting experience, we propose to simulate those measurements by employing the physically based model CATFLOW (2d Richards-Eq.). Those constitutive relations where derived for a concrete catchment, the Weiherbach catchment. In this catchment we have an excellent database and we know which model structure gives good results for reproducing discharge, soil moisture and ET measurements over a long period. We propose to use this model structure to simulate hillslope scale drainage and wetting experiments. We average capillary pressure, saturation over the entire hillslope volume and the out- or inflow (depends on drainage or wetting case) over the lower boundary. In a next step we use this time series of REW scale average properties/fluxes select Brooks and Corey type relations.
and fit parameters.

This is essentially the same procedure that is applied to fist size soil sample for deriving soil hydraulic functions. In the paper we show, that different hillslope scale patterns of soils result in different curves and different parameter. Thus, as in the case of soil samples, the parameters embed the effect of subscale structures in the textural parameters at the next higher scale (in the sense of the scale way concept of Vogel and Roth, 2003). The nice thing is, that the parameter values we obtain for the model structure, that yielded reproduction of observed dynamics in the Weiherbach catchments, are pretty close to those Haksu Lee obtained, when calibrating this constitutive relations within a successful application of the CREW model (which is an implementation of the REW equations into a code) to the Weiherbach catchment, that yielded simultaneously a good reproduction of observed discharge and soil moisture data.

Keith Beven: Then there is the question of equifinality that is also neglected in these papers. OK, so the results presented in reproducing soil and discharge responses are “reasonable” (though they would not appear to be really acceptable yet in reproducing either discharges or soil water dynamics). But is it not a concern that there might be many other possible forms and parameter sets that would do equally well? And since the results are not actually that good, should there not be some concern about uncertainty in parameters (and, indeed, measurements)?

Response: Within his application of CREW of 0.8 with a single REW for the Weiherbach catchment. Furthermore the time series of u-zone saturation is enveloped by observations of soil moisture at 61 points (data time step is 2 weeks) and shows a good agreement with the time series of soil moisture that was derived by averaging the fields generated with CATFLOW within a simulation for the same period. We call this acceptable (Zehe et al. 2001, Zehe and Blöschl, 2004)!

We do not neglect equifinality in this paper. However, we do not think that this is quite the write term when dealing with spatially highly resolved models, data, because
these models may resolve spatial patterns. We think that Keith Beven is referring to the uncertainty/ or heterogeneity of spatial patterns of key features such as saturated hydraulic conductivity and macropores. In the new manuscript we investigated the effect of heterogeneity of soil hydraulic conductivity and macroporosity. To this end we compared 4 cases - The normal hillslope catena with homogeneous soils - The normal hillslope catena + a heterogeneous pattern of ks generated with turning bands (total variance was estimated based in field data to 1 order of magnitude) - The normal hillslope catena + a heterogeneous pattern of ks + a typical pattern of discrete macropores (generated with a poission process, data taken from field investigations). As observed in the Weiherbach the macropores penetrate in average 0.8 m into the depth and end in the soil matrix. - The normal hillslope catena + a heterogeneous pattern of ks + a deep pattern of discrete macropores (generated with a poission process, data taken from field investigations). In this case the macropores penetrate the lower boundary of the modelling domain, hence drainage from those macropores is not controlled by the soil matrix at their end.

As the graphs in the end show, the first three model structure yield the same spatially average outflow after a total averaging length (REL) of 50 m, which is app. 0.25 of a typical Weiherbach slope. Only the forth case gives, as expected different spatially averaged outflow values. This shows: there is an REA/REL for the Weiherbach, were drainage into the s-zone can be treated homogeneous. This shows furthermore, that the average value embeds information on the spatial connectivity of macropores /structures with them at the next higher scale, as the 4th case yields a clearly higher average outflow. However, case 4 is not the relevant for the Weiherbach catchment as earthworm burrows there never penetrate down to the saturation zone (which is located between 3 and 30 m.

Keith Beven: In this respect the authors have only taken part of the uniqueness of place argument on board. This did not say that uniqueness of place would preclude extrapolation of parameter sets as prior estimates. It did say that it should be expected that
those prior estimates would be highly uncertain (partly because of interactions amongst parameters in the set means that there is a need to drift behavioural sets of parameters from gauged sites to ungauged sites) and that we should therefore aim to reduce that uncertainty by appropriate measurement where possible (and that some types of data collection might prove to be much more valuable than others in that respect). It is these issues that are the really exciting essence of the potential advances to be made in the REW theory. The REW concepts should be used for formulating something new - NOT seeing if we can get away with doing the same thing over again (but in one sense badly in the sense that the current solutions in CREW etc will be a poor approximation to (and may not be convergent with) the true solution of a continuum Richards equation in a heterogeneous domain (before even considering preferential flow effects).

Response: It was not our purpose to abuse the uniqueness of the place idea, which is very valuable!! The point we wanted to make was that for setting up the model structure for the simulated wetting and drainage experiments we used knowledge/understanding about unique or typical features of the Weiherbach catchment e.g. the knowledge how the catena looks like and that earth worm burrows do not penetrate into the saturated zone. (Please note that this makes the difference between case 3 and 4). So our question to which extend those constitutive relations are only valid for the Weiherbach catchment is, from our point of view appropriate. By adopting the pattern-process-paradigm from theoretical ecology we argue that the hillslope soil catena in as well as the fact that earthworm do not penetrate through the huge loess layers is typical for the whole Kraichgau, which is the landscape unit the Weiherbach is located in. We argue that the constitutive relations might be therefore also typical for this landscape and might be adopted for modelling exchange processes between the unsaturated zone and the saturated zone. We consider REW derived for the Weiherbach catchment therefore as a functional unit for building mesoscale models in this landscape. In the new manuscript we omit the reference to uniqueness of the place, as it was not found to be feasible by Keith Beven.
Some further specific quantities:

Keith Beven: p.3: state variables must be measurable quantities. ???? in what sense is this possible for any distributed model element or REW???.

Response: The statement is in fact: meaningful state variables and parameters that may be derived from field observations using appropriate upscaling. We are aware that is currently not possible to observe states in the unsaturated zone at the REW scale. It might be already the case for piezometer heads in the saturated zone (depending of the support of a single measurement). That’s why we add the term upscaling, e.g. by employing a physically based distributed model as interpolator (in the sense specified in the paper.) Let’s argue from the other side: If we ever succeed in assessing observations of REW/catchment scale state variables, states produced by models should of course be compatible with those observations. Besides the REW approach I see currently not a single model in the market place that could meet this condition.

Keith Beven: p.3 using appropriate upscaling. ??? how is this going to be possible. Upscaling will be predicated on knowledge of small scale properties that we will never ever have?? Response: Upscaling from the pore to the REV scale for deriving soil hydraulic functions is possible as e.g. by Vogel et al.(2005 VZJ) if the necessary information about interconnected structures are available and they are represented within a model. Upscaling in the Weiherbach is, partly, possible if information about structures are macropores are available as it is the case for the Weiherbach (compare cases 1-3).

Keith Beven: p.5. “texture” at the REW scale will certainly be important - but you then neglect any consideration of texture later in this paper where parameters are assumed to be homogeneous “effective” values. Response: Dynamics in a texture at any scale will always be described using continuum mechanics. We can account for subscale heterogeneity in a statistical sense, but not explicit anymore. An REW is the smallest unit, which is not further resolved. Per definition it has to be described using continuum mechanics and parameters that parametrise subscale structures. Lets think about two
grid cells at the REV scale, one represents a sandy soil the other a clay. Both get homogeneous parameters, but they are different and represent the effect of subscale structures. For the case of the REW it is the same. We could additionally account for subscale heterogeneity within the REW, and this would be of key importance for transport issues, but only by linking the REW approach with stochastical approaches e.g. to predict the pdf of residence times.

Keith Beven: p.8. simulated state variables are physically consistent with local observations—simulated time series of catchment average soil moisture and matric potential may be used as target measures for validation of meso-scale models. How can this be acceptable? Local soil moisture measurements are not commensurable with what you are predicting, nor is Figure 4 compelling as evidence of physical consistency - surely many other formulations would seem equally plausible (even a simple mean value!). Response: Figure 4 has to be interpreted with Figure 3. In Figure 3 we show that a simple re-arrangement of hillslope scale soil and macroporosity pattern always leads to a bad model performance. Those model structures are not acceptable, please compare the simulated flood event. The structure we call landscape and process compatible yields the best match. In Figure 4 we show that those re-arranged patterns yield a total different time series of the average catchment scale saturation in the unsaturated zone. Figure 4 shows in the lower panel that the time series of average catchment scale saturation simulated with the landscape and process compatible model structure is enveloped by the measurements. Hence, we claim that this time series, which corresponds to a model structure that a) explicitly represents patterns we observed in the Weiherbach b) yields simulation results which match on the long term ET, discharge and soil moisture well (as stated in the text, and which is enveloped by the observations is a physically consistent estimator for catchment scale average soil saturation in the u-zone. Physically consistent because we average the output of the model which is based on soil physics. Keith Beven might be right that there could be different model structures which would produce the same results. However, as physically based models are spatially explicit we are not interested in assessing those
structures. We have observed information (Zehe and Blöschl, 2004, WRR) about soil patterns, macroporosity, soil hydraulic functions etc. which already allow us to reject a lot of possible model structures a priori. The model structure we end up with fits to the landscape (our observations) and to the observed dynamics. I strongly doubt that we would find many more model structures different from the one we call landscape and process compatible one that meets both conditions. As can be seen in Fig.3 and 4 a little disturbance of the patterns of soil and macropores already lead to a much worse model performance.

Keith Beven: p.10. Equations 5. should there not be some consideration of hysteresis at larger scales (over an above that due to local scale hysteresis and the effects of macropores)? Response: We investigated the effect of macropores on the drainage and wetting experiments in case 3 and 4 in the new manuscript, It has only an effect if the macropores penetrate through the model domain! However, as already stated, above this not relevant for the Weiherbach; the worm burrows never reach the saturated zone there. Hysterisis???

Keith Beven: p.11. There is a long history of work that suggests that infiltration excess overland flow cannot be predicted by homogeneous effective soil properties - trying to do so means that surface runoff contributing areas are either 0 or 100% of the REW. Response: As this study does not present any model results with a model based on the REW approach, I am not sure what the comment is aiming at. It is of course possible to simulated Hortonian overland flow with spatially distributed physically based models and account for runoff coefficients smaller than 100% (Zehe and Blöschl, 2004 WRR).

p.15. the units of macropore volumes might be better stated as m3m-2 if that is what the authors meant.

Keith Beven: p.20. 95% confidence limits. Not clear how these are estimated (reference to Eqn. 5 misleading as these are not stochastic). Response: (Non) linear regression parameters get always confidence limits, e.g. because of the fact that the sample is finite, this is standard univariate statistics (e.g. Hartung, Lehrbuch der Statis-
tik). Our suggestion is that one could use these limits for constraining model parameter ranges when the model uncertainty is quantified e.g. using the Glue approach.

Keith Beven: R2 of 0.51 seems to be cited as 0.98 in Table 2 (or I may be missing something??)

Keith Beven: p.23. This is a misrepresentation of the uniqueness of place arguments (see comments earlier). The authors need to think much more about the uncertainty with which the properties of any particular landscape can be estimated. In addition, the idea that landscapes are in equilibrium states cannot be supported by the evidence over large parts of the globe (surely including the Weiherbach catchment, where I would suspect that there is still evidence of glacial and periglacial processes affecting the soils and bedrock properties). This discussion should be cut.

Response: It was not our purpose to abuse the uniqueness of the place idea, which is very valuable within this study. The point we wanted to make was, that for setting up the model structure for the simulated wetting and drainage experiments we used knowledge/ understanding about unique or typical features of the Weiherbach catchment e.g. the knowledge how the catena looks like and that earth worm burrows do not penetrate into the saturated zone. (Please note that this makes the difference between case 3 and 4). So our question to which extend those constitutive relations are only valid for the Weiherbach catchment is, from our point of view appropriate. By adopting the pattern-process-paradigm from theoretical ecology we argue that the hillslope soil catena in as well as the fact that earthworm do not penetrate through the huge loess layers is typical for the whole Kraichgau, which is the landscape unit the Weiherbach is located in. We argue that the constitutive relations might be therefore also typical for this landscape and might be adopted for modelling exchange processes between the unsaturated zone and the saturated zone. We consider REW derived for the Weiherbach catchment therefore as a functional unit for building mesoscale models in this landscape.
Keith Beven: In conclusion, I must emphasise that am not criticizing the REW concepts. I have argued strongly in several papers that the future of hydrological modeling lies with the REW concepts. This is because of the way in which the REW approach allows a new look at the problem of representing the effects of complexity at the scale of discrete REW landscape units (for which a representation of fluxes based on continuum mechanics will not be appropriate). There is still nothing wrong with the concepts, but, while recognizing that the implementation of closure schemes is a very difficult problem, there is a lot in this paper (and, it must be said, in other recent applications of the REW concepts) that is totally incompatible with the fundamental principles of the REW approach. The only justification for not requiring a major revision of this paper is the argument (made cogently by Siva elsewhere) that to learn from applying those concepts we have to start somewhere. That is a decision for the editors. My own contribution to the REW special issue (see HESSD-2006-0009) expresses the opinion that this is not a strong enough argument. It is analogous to saying that if we set off up a one way street in the wrong direction it will eventually get us to our destination. We can already perceive what that destination should look like, and I would suggest that this paper is not heading in the right direction.

Final response: We of course disagree. Concerning the Keiths own paper (Searching for the holy grale in scientific hydrology) we just want to admit that: closure is nothing like a saturation-discharge relation per se, but always related to a equation (which we miss thereÊ). But this is not about his but about our paper. We think that the presented approach gives suitable constitutive relations for modelling the Weiherbach catchment. We don’t think that there is a single way to solve the closure problem, there will be for sure many ways, and the use of physically based models for assessing closure relations reasonable (in the sense of Vogel and Roth, 2003), by the way this is also done in boundary layer meteorology. We think the presented results give evidence that the effect of subscale patterns and structures can be embedded within texture at the next higher scale, that these relations yield simulations which match observations well, when used within the application of the CREW model to the Weiherbach catchment.
(see Lee et al. 2006 HESS this issue). We admit, that the study could be advanced. One way is go beyond just accounting for average flow in the unsaturated zone, but to model the whole distribution. The other would be to further investigate the effect of hysteresis. However, as Keith pointed out, one has to start somehow!

Please find the mentioned figures below

Figure 2: Hillslope scale model structures for investigating the effect of small scale heterogeneity on the numerical experiments. Upper left panel is case 1 typical soil pattern with Calcaric Regosol in the upper part 80% and Colluvisol in the lower 20%, the corresponding values of the saturated hydraulic conductivity are given in Table 1. Upper right panel is the same soil pattern as in case 1 which is superimposed by a stochastical field of saturated hydraulic conductivities generated with turning bands. Case 3 in the lower left panel same structure as in case 2 but that contains a population of macropore that is typical for the Weiherbach catchment generated with a poison process. Case 4 in the lower left panel same structure as in case 2 but that contains a population of macropore that is not typical for the Weiherbach catchment generated with a poison process. The macropores penetrate through the lower boundary of the domain.

Figure 5: Outflow across the lower boundary averaged over different fractions of the lower boundary, starting at the lower left corner (averaging length is zero) up to the full extend (averaging length is 100 m i.e. the total lower boundary). The upper left panel is case 2, the upper right case 1, the lower left belongs to case 3 and the lower right panel to case 4

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