Regionalization of Subsurface Stormflow Parameters of Hydrologic Models:
Up-scaling from Physically Based Numerical Simulations at Hillslope Scale

Melkamu Ali¹, Sheng Ye², Hong-yi Li³, Maoyi Huang³

L. Ruby Leung³, Aldo Fiori¹ and Murugesu Sivapalan^{2, 4}

Submitted to *Journal of Hydrology*

June 30, 2014

Abstract

Subsurface stormflow is an important component of the rainfall-runoff response, especially in steep forested regions. However; its contribution is poorly represented in current generation of land surface hydrological models (LSMs) and catchment-scale rainfall-runoff models. The lack of physical basis of common parameterizations precludes *a priori* estimation (i.e. without calibration), which is a major drawback for prediction in ungauged basins, or for use in global models. This paper is aimed at deriving physically based parameterizations of the storage-discharge relationship relating to subsurface flow. These parameterizations are derived through a two-step up-scaling procedure: firstly, through simulations with a physically based (Darcian) subsurface flow model for idealized three dimensional rectangular hillslopes, accounting for within-hillslope random heterogeneity of soil hydraulic properties, and secondly, through subsequent up-scaling to the catchment scale by accounting for between-hillslope and within-catchment heterogeneity of topographic features (e.g., slope). These theoretical simulation results produced parameterizations of the storage-discharge relationship in terms of soil hydraulic properties, topographic slope and their heterogeneities, which were consistent with results of previous studies. Yet, regionalization of the resulting storage-discharge relations across 50 actual catchments in eastern United States, and a comparison of the regionalized results with equivalent empirical results obtained on the basis of analysis of observed streamflow recession curves, revealed a systematic inconsistency. It was found that the difference between the theoretical and empirically derived results could be explained, to first order, by climate in the form of climatic aridity index. This suggests a possible co-dependence of climate, soils, vegetation and topographic properties, and suggests that subsurface flow parameterization needed for ungauged locations must account for both the physics of flow in heterogeneous landscapes, and the co-dependence of soil and topographic properties with climate, including possibly the mediating role of vegetation.

Keywords: subsurface flow, soil and topographic, heterogeneity, closure relations, storage-discharge relationship, statistical methods, Richards equation, up-scaling, climate

1. Introduction

Due to high infiltration capacities of the soil, steep slopes, and the presence of macropores that enhance downslope water movement, subsurface stormflow is a dominant streamflow generation mechanism in steep forested regions of the world (McDonnell, 1990; Sidle *et al.*, 2000; Fiori, 2012). However, its contribution is poorly represented in the current generation of land surface hydrological models (LSMs) and catchment-scale rainfall-runoff models. Most LSMs incorporate the role of the subsurface stormflow using various forms of parameterizations (Lee *et al.*, 2005; Yeh and Eltahan, 2005; Huang and Liang, 2006; Huang *et al.*, 2008). The lack of physical basis of most common parameterizations precludes *a priori* estimation (i.e. without calibration) and has provided the motivation for much research focused on the role of subsurface stormflow and groundwater dynamics on the simulation of land surface water and energy fluxes in climate models.

Recent work by Hou *et al.*(2012) and Huang *et al.*(2013) has shown that water and energy flux predictions at the land surface with the CLM4 model were most sensitive to the subsurface runoff parameterizations (see also Niu *et al.*, 2005; Niu *et al.*, 2007). Most current LSMs do not fully account for the contribution of subsurface stormflow to total streamflow and parameters that represent subsurface stormflow are not physically based. For example, the ARNO formulation of subsurface flow (Todini, 1996), which is also embedded in the variable infiltration capacity (VIC) model (Liang *et al.*, 1994), is empirically based and lacks physical grounds for establishing the associated parameters, which limits its extension to predict in ungauged catchments (e.g., Huang and Liang, 2006). On the other hand, most existing models of subsurface stormflow from hillslopes and small catchments are based on analytical solutions to the Boussinesq equation assuming equivalent representative values of catchment properties (e.g., Brutsaert and Nieber, 1977; Brutsaert and Lopez, 1998; Rupp and Selker, 2005; Rupp and Selker, 2006). This critical review points to limitations of parameterizations of subsurface flow in current LSMs; the intention of this paper is to explore alternative approaches towards the improvement of subsurface flow parameterizations in both rainfall-runoff models and LSMs, including how to embed the effects of subsurface heterogeneity in a physically based manner.

This paper is the second of a two-part paper aimed at deriving physically based storage-discharge relations as parameterizations of subsurface stormflow, which can then be embedded in land surface models without the need to resolve the flows at smaller scales explicitly. We are looking for a catchment-scale parameterization of the form:

$$Q = a S^b \quad (1)$$

with parameters a and b that are meant to capture the net effects of the heterogeneity of soil and topographic properties. Along the way, the paper aims to (1) identify the most important landscape controls on the storage-discharge relationship and (2) use these to develop a simple prediction equation on the basis of measureable landscape characteristics that could be applied to ungauged basins on a regional basis.

One approach to developing such parameterizations is to infer these, using an inverse procedure, from catchment runoff measurements that already account for the net effects of natural variability of soil and topographic properties. It is straightforward to show that the parameters a and b of the storage-discharge relationship can be related to the parameters α and β associated with the recession slope curves (see also Ye et al., 2013):

$$\alpha = a^{1/b} b \quad (2a)$$

$$\beta = 2 - 1/b \quad (2b)$$

where the parameters α and β govern the shape of the recession-slope curve extracted from observed streamflow records. The recession-slope curve, defined by Brutsaert and Nieber (1977), describes the slope of the recession curve after cessation of rainfall, $-dQ/dt$, as a function of discharge Q , in terms of a power-function, as follows:

$$\frac{dQ}{dt} = -\alpha Q^\beta \quad (3)$$

In an accompanying paper, Ye *et al.* (2013) adopted an empirical analysis approach that capitalized on the use of recession-slope curves to derive the storage-discharge relationship. However, runoff measurements are limited to a few locations, and due to the high spatial variability of the factors that contribute to subsurface stormflow, some of which are not easy to

measure, it is not straightforward to extrapolate such empirical relationships from gauged locations to ungauged ones. An alternative approach to developing these parameterizations is to use numerical simulation approaches with the use of detailed physically based hydrological models that account for known or assumed forms of spatial variability of soil and topographic properties (Robinson and Sivapalan, 1995; Duffy, 1996; Viney and Sivapalan, 2004; Lee *et al.*, 2005). The present study falls in this latter area and builds on considerable prior research activity.

A recent study by Fiori and Russo (2007) used a three dimensional numerical model to study flow in heterogeneous hillslopes and found that discharge in the presence of heterogeneous soils is always larger than for homogeneous media with equivalent properties. Harman and Sivapalan (2009b) investigated flow through heterogeneous hillslopes and showed that the presence of heterogeneity produced responses fundamentally different from hillslopes with homogeneous soils. The role of topographic variability in controlling subsurface responses at the hillslope scale has also received increased attention in recent times (Freer *et al.*, 1997, Troch *et al.*, 2002, 2003; Bogaart and Troch, 2006; Fujimoto *et al.*, 2008) since it has a considerable impact not only on the short-term dynamics of streamflow and spatial patterns of soil moisture, but in the long term it also impacts the spatial patterns of soil and vegetation properties (Bachmair and Weiler, 2012).

The present study is different from previous research in several respects: (i) it aims to derive physically based parameterizations of subsurface stormflow at the catchment scale, accounting for the effects of heterogeneity of both soil hydraulic properties and topographic slope; (ii) the two-stage up-scaling procedure adopted here (from point to hillslope, and from hillslope to catchment scales) is implemented in a comparative manner in 50 actual catchments; (iii) the parameters of the derived power-law storage-discharge relationships (a and b) are converted to (α and β) and then regionalized through derivation of multiple regression relationships with landscape soil and topographic properties, and these are then compared against corresponding expressions derived through empirical recession curve analyses on the same 50 catchments (Ye *et al.*, 2013). In other words, the two studies approach the problem of subsurface flow parameterization from both bottom-up (this study) and top-down (Ye *et al.*, 2013) perspectives.

2. Up-scaling methodology and data resources

The goal of this study is to derive catchment-scale closure relations in the form of storage-discharge relations at steady state that account for the net effects of spatial heterogeneity of landscape characteristics (i.e. soil hydraulic properties and topographic slope). The heterogeneity of landscape properties can be highly complex, multi-scale, and much of it (relating to the soils) unknown. For the purpose of this study we simplify the heterogeneity, without loss of generality, by considering two kinds of spatial heterogeneities: (i) within-hillslope soil heterogeneity (both random and deterministic), while topographic slope is assumed to remain uniform within the hillslope, and (ii) between-hillslope heterogeneity of topographic slope, whereas the nature of soil heterogeneity is assumed to be the same (and repeated) between hillslopes. In other words, the building blocks of the up-scaling analysis will be the population of hillslopes that constitute a catchment; for simplicity, the hillslopes will be assumed to be planar and rectangular.

Given the nature of spatial heterogeneity assumed above, the proposed work involves a two-step up-scaling procedure: (i) from the point (or local) scale to the hillslope scale, to account for within-hillslope soil heterogeneity, maintaining constancy of hillslope topography, and (ii) from the hillslope to the catchment scale (using parameterized forms of the previous up-scaling to the hillslope scale), now accounting for between-hillslope variability of topography within a catchment. The first step of the up-scaling is carried out with the use of numerical simulations of the Richards' equation at the hillslope scale, which are repeated for several cases by varying the topographic slope and soil hydraulic properties, including different levels of their heterogeneity. Under steady state conditions (i.e., recharge equaling discharge), for all combinations of topographic slope and soil properties, hillslope-scale storage-discharge relations are derived, and expressed in a power-law form. The results of these multiple simulations are pooled together, and regression relationships are derived for the parameters of the storage-discharge relations (i.e., coefficient a and exponent b , but at the hillslope scale only) in terms of the controlling soil and topographic properties. Together, these constitute parameterizations of hillslope-scale storage-discharge relations at steady state. The summary results arising from the first up-scaling step to the hillslope-scale are then up-scaled again to the catchment scale, through the application of the “disaggregation-aggregation approach” proposed by Sivapalan (1993) and Viney and

Sivapalan (2004) to account for the effects of between-hillslope heterogeneity of topographic slopes.

The proposed two-step up-scaling procedure is implemented in 50 catchments in eastern United States, which are a subset of the much larger MOPEX dataset (Duan et al., 2006), generating power-law form storage-discharge relationships for each catchment (and associated coefficients and exponents). Regional relationships are derived for the coefficient and exponent of these storage-discharge relationships in terms of measured topographic and soil hydraulic properties also at the catchment scale. These are then compared against corresponding regional relationships derived from observed streamflow recession curves for the same 50 catchments, carried out as part of the parallel study by Ye *et al.* (2013).). These 50 catchments were chosen under the criteria to minimize the influence from other confounding factors: reasonable number of flow events, minimal impact of regional groundwater and/or snowmelt, minimal human impact and maximum data availability, especially soils data.

2.1. Up-scaling to the hillslope scale: numerical simulations

For the first up-scaling step, we simplify each hillslope as a heterogeneous planar, rectangular hillslope of specified length, width and depth, and specified constant topographic slope. Within each hillslope, we assume an idealized form of the heterogeneity of the surface soil hydraulic conductivity, in the form of a correlated random field in 2-D. In addition to the horizontal, random heterogeneity, the saturated hydraulic conductivity is also assumed to exhibit a further (deterministic) vertical decrease with soil depth.

It is assumed that the 2-D field (i.e., planar, along hillslope surface) of the saturated hydraulic conductivity, K_s , is a stationary and isotropic field following a log-normal probability density function (i.e. $Y = \ln(K_s)$ is Gaussian), with assumed known mean $\langle Y \rangle$, variance ($\sigma_{\ln K}^2$) and correlation length (l). We kept other properties such as porosity constant and focus only on the spatial heterogeneity of K_s . We further assume that the random field Y has an exponential auto-covariance structure (El-Kadi and Brutsaert, 1985; Fiori and Russo, 2007) given by

$$C(\xi) = \sigma_{\ln K}^2 \exp\left(-\frac{\xi}{I}\right) \quad (4)$$

where C is the covariance function; $\sigma_{\ln K}^2$ is the variance; I is the correlation length and $\xi = x - x'$ is the separation vector. For the characteristic hillslope length scale L , we choose the correlation length such that $I/L = 0.04$ consistent with the scale of the problem, with the domain being discretized into equal cells measuring $\Delta x_1/L = \Delta x_2/L = 0.005$ in the horizontal and $\Delta x_3/L = 0.0025$ in the vertical.

The numerical simulations of three-dimensional, saturated/unsaturated flow in heterogeneous porous formations are rather complex and typically require a large computational time. The number of cases to be examined is also large, of the order of 2000. In order to reduce both the computational time and the total number of simulations, we have adopted the single realization approach by Fiori and Russo (2007); the latter consists of employing a flow domain which is large enough to warrant ergodicity, such that the results of the simulations adequately represents the ensemble statistical properties of the flow variables, but not too large, to limit the computational time. Thus, the choice of the domain size results from a tradeoff between computational time, number of simulations to be performed and the ergodicity requirement. The single realization of the saturated hydraulic conductivity field used in the simulations was generated using HYDRO_GEN (Bellin and Rubin, 1996) and then rescaled in order to respect the constant mean saturated hydraulic conductivity of the surface.

The variation of saturated hydraulic conductivity variation along the vertical direction is assumed to be deterministic, with a decrease with depth reflecting, amongst other factors, the result of compaction and differential weathering. Following Beven and Kirkby (1979), Beven (1982) and Sivapalan *et al.* (1987), for simplicity, we assume an exponential decrease given by:

$$K_s(z) = K_0 e^{-fz} \quad (5)$$

where $K_s(z)$ is the saturated hydraulic conductivity at depth z measured from the soil surface, K_0 [LT^{-1}] is the saturated hydraulic conductivity at the soil surface, which has been previously generated by the random field generator, and f [L^{-1}] is an exponential decay parameter.

Subsurface flow within the hillslope is assumed to be governed by the three dimensional Richards' equation with the focus on saturated flow dynamics only (see Appendix A for the details of the Richards equation formulation used). The initial condition is one where the water table is at the surface and the system is fully saturated. The upper boundary condition is an assumed net precipitation. A no-flow boundary condition is assumed at the bottom; the same is true for the right, left and the back vertical planes parallel and normal to the flow direction. A seepage face is assumed at the front vertical boundary through which water discharges to the stream. During the simulations, under the assumed precipitation input, the hillslope drains down from its initial totally saturated condition, to a steady state condition commensurate to the applied precipitation or recharge rate.

A dimensionless form of Richards' equation is solved by the finite element method using the earth science module of Comsol Multiphysics software that employs numerical methods to solve partial differential equations (COMSOL AB, 2010). So long as the boundary conditions and the ergodicity assumptions continue to hold, the dimensionless results from the simulations can be rescaled back to obtain results for variable hillslope lengths and depths, as needed for extension to heterogeneous catchments. In order to obtain the S-Q relationship, we have performed a set of numerical simulations with different topographic, soil properties and recharge. Each steady-state simulation was carried out by using full initial saturation conditions, imposing a given recharge (equal to the desired discharge), and performing a transient simulation until steady state is reached. The saturated storage is recorded at the end of the simulations. The same procedure is repeated for several values of the recharge, topographic slope and soil properties in order to produce the required steady-state storage discharge curves.

The ultimate result we are looking for at the end of the first-step of the up-scaling procedure is the hillslope-scale storage-discharge relationship, $Q_i(S_i)$, for a given hillslope i within a catchment, expressed in the form:

$$Q_i = Q_i(S_i) = a_i S_i^{b_i} \quad (6)$$

where Q [L^2/T] is the discharge from the hillslope per unit width of stream and S [L^2] is the saturated zone storage within the hillslope (also per unit width), and the coefficient a_i and the exponent b_i are constants that reflect the soil and topographic properties of hillslope i .

Although the limitations of the assumptions we have made in this modeling approach and the parameterization of the storage-discharge relationship have been well documented in the literature, it is essential to re-emphasize these here to make sure that our approach can be extended further in the future to enable it to be applied to any ungauged basin, regardless of the specific hydrological characteristics. Some of the limitations and possible remedies for these are: (1) steady-state assumption for the Q-S relation is similar to the widely employed kinematic modeling, in which the continuity equation is coupled with a simplified dynamic formula based on steady-state and it is normally considered an appropriate way of simplifying the model structure and parameterizations. However, the steady state assumption may not be applicable in some cases since recharge rate can be spatially non-uniform and may change over time during a rainstorm and inappropriate for the upslope zone where the saturated depth of the aquifer is large which produces a large deviation of the actual water table from the steady state shape, as shown by Seibert et al. (2003) and Sloan (2000). (2) The derived storage-discharge relationship is based on the assumption that saturated hydraulic conductivity varies exponentially with depth, which may not be valid for a very shallow soil layer. However, it should be noted that Beven (1982) summarized results from a number of field studies on the variation of saturated hydraulic conductivity with depth, which showed that the exponential decay is a reasonable way to describe this dependency. The decrease of K_s with depth may also mimic the presence of discontinuities in the soil-subsoil interface, where the latter is usually less permeable. Hence, it is a convenient and parsimonious way to model vertical contrasts of K_s . A similar procedure is adopted in our model formulation here, rendering the resulting solutions generally applicable. (3) The assumption that capillarity effects in the unsaturated zone above the phreatic layer can be neglected. In a situation where capillary effects need to be considered, a simple correction term can still be adopted, such as the approach introduced by Parlange and Brutsaert (1987) in the context of their kinematic model. However, these extensions are beyond the scope of this paper.

2.2. Derivation of parameterizations of storage-discharge relations

Upon completion of numerical simulations for a large combination of soil and topographic properties, we use variable selection methods to develop empirical relationships between the parameters of the storage-discharge relationship (coefficient a and exponent b) and the landscape (soil and topographic) properties. This is to ensure accurate prediction with a small set of variables that are shown to significantly impact the storage-discharge relationship. The predictor variables include: (1) variables that define the soil hydraulic properties and their spatial variability along the horizontal and vertical soil profiles, and (2) variables that define the hillslope geomorphology, particularly topographic slope.

We first study the influence of each landscape property and their individual effect on subsurface flow and storage, and the storage-discharge relationship. This is done through sensitivity analyses with the simulation model for different combination of predictor variables. Topographic slopes of individual hillslopes were specified as 5, 10, 20, and 30°; the mean surface hydraulic conductivity (K_s) values used ranged from 3 to 42 $\mu\text{m/s}$ with horizontal heterogeneity ranging from homogeneous to strongly heterogeneous ($\sigma_{\ln K}^2 = 0.0, 0.5, 1.0$ and 2.0); the range of values of the vertical decay parameter, f (m^{-1}), were chosen such that $fd = 0.0, 1.25, 2.5$ and 5.0. The equilibrium (steady-state) subsurface storage under a range of steady recharge values were computed for these various parameter combinations.

Upon completion of the simulations and the derivation of storage-discharge relations expressed in power-law form, $Q_i = a S_i^b$, we used multiple variable regression to develop functional relations relating the parameters a and b (or their logarithmic forms) to the chosen predictor variables. Several regression equations were developed with the combination of the predictor variables involved in the numerical simulation and then the best model was selected based on the Akaike Information Criterion (AIC), which is a measure of the relative goodness of fit used to choose the most suitable model with least information loss (Akaike, 1974), with a penalty term included to constrain increase in model size (2k). Since we have a small number of samples in our study, a second order bias correction for AIC was adopted (Sugiure, 1978). This criterion is denoted as AICc to make it distinct from AIC and was computed using the following equation,

$$AICc = AIC + \frac{2k(k+1)}{n-k-1} = -2\ln(L) + 2k + \frac{2k(k+1)}{n-k-1} \quad (7)$$

where $\ln(L) = -(n/2)\ln(RSS/n)$ is the maximum log – likelihood, n is the sample size and k is the number of predictors used in each model, RSS denotes the residual sum of squares from the value of the response (i.e. a or b or their logarithm forms) predicted by the fitted model. Furthermore, adjusted R^2 was used to assess the performance of the models compared to the estimated values from the numerical dataset:

$$R_{adj}^2 = 1 - \frac{SSE}{SST} \frac{n-1}{n-k-1} \quad (8)$$

where SSE is the sum of squared errors and SST is the total sum of squares.

2.3. Up-scaling to catchment scale: disaggregation-aggregation approach

Given the results from the earlier up-scaling, we now need another up-scaling step to extend the hillslope scale parameterization of subsurface stormflow all the way to the catchment scale. For simplicity, especially for computational reasons, we will not undertake numerical simulations of the Richards' equation at the catchment scale to account for both soil and topographic heterogeneity (even though this is technically feasible). Instead, the approach adopted for up-scaling involves dividing a catchment into a large number of representative elementary catchments, each of them being further divided into two or more hillslope building blocks. The parameterizations obtained in the previous step at the hillslope scale are then implemented for the individual hillslopes, and the results aggregated up to the catchment scale. Figure 1 presents a schematic that illustrates the implementation of the up-scaling strategy.

The proposed up-scaling strategy is subject to a number of simplifying assumptions; 1) natural hillslopes in the catchment are all rectangular shaped (Figure 1) draining to the intermediate stream within each elementary watershed from both sides, and in the case of elementary first order watersheds, a hillslope that drains towards the source node, 2) the effects of natural heterogeneity of soil properties (i.e., saturated hydraulic conductivity) on subsurface flow within hillslopes are fully parameterized, with any between-hillslope heterogeneity of soil properties assumed negligible; and, 3) the only heterogeneity that remains between hillslopes is topographic, and here we assume that only the topographic slope and hillslope length are

variable between hillslopes and all other geometric properties remain constant. Clearly, these are strong assumptions but are made to keep the problem tractable. Future work, especially when more information is available on soil properties, can relax these assumptions, and provide more refined and realistic results. It is pertinent to note here that the assumption of rectangular and planar hillslopes is a gross simplification, considering that there is literature pointing to the importance of the shapes of hillslopes in plan and in elevation (convex/concave, converging/diverging) on the dynamics of subsurface stormflow and surface saturation (O'Loughlin, 1981; Troch et al., 2002, 2003). It is left to future research to address the issue of corrections that need to be made to the storage-discharge parameterizations.

The up-scaling problem can now be framed as follows: given the storage S at the catchment scale, what is the corresponding discharge, Q ? Or, what is the storage-discharge relationship at the catchment scale, $Q = a S^b$, and how can we derive this on the basis of the hillslope-scale storage-discharge relationship $Q_i = a S_i^b$ derived earlier for individual hillslopes? In this paper the up-scaling is carried out using the disaggregation-aggregation approach proposed by Sivapalan (1993) and Viney and Sivapalan (2004). Assuming quasi-steady state, given the catchment-scale discharge Q , this is disaggregated to recharge (equal to discharge) per unit area $q = Q/A$, where A is the catchment area. Given this recharge rate per unit area, for a given hillslope i , the steady discharge rate per unit stream width is $Q_i = A_i q$, where A_i is the hillslope area per unit stream width. We can then estimate the hillslope scale storage S_i , corresponding to Q_i , through the inversion of the hillslope-scale storage-discharge relationship presented in Eq. 5 above for that hillslope. The catchment-scale water storage can then be obtained through the aggregation (as a weighted average) of all of the hillslope-scale storages, S_i , for all of the hillslopes i constituting the whole catchment, as follows:

$$S = \sum_{i=1}^n \frac{A_i}{A} S_i(Q_i) = \sum_{i=1}^n \frac{A_i}{A} \left\{ \frac{A_i}{a_i} \frac{Q}{A} \right\}^{1/b_i} \quad (9)$$

This estimation procedure is repeated for different values of catchment scale discharge, Q , and in this way the storage-discharge relationship at the catchment scale is derived.

2.4. Implementation in actual catchments: MOPEX dataset

The up-scaling procedure presented above is implemented in 50 catchments belonging to the Model Parameter Estimation Experiment (MOPEX) dataset, mostly in the East and Midwest of the United States (see Figure 2a). Topographic slope, aridity index (AI, which is the ratio of mean annual evaporation to mean annual precipitation), drainage density, mean and standard deviation of saturated hydraulic conductivity at the surface, the vertical (exponential) decay parameter of the saturated hydraulic conductivity, soil porosity, soil depth and drainage density were extracted and calculated for these 50 catchments from MOPEX, NHD, and NRCS SSURGO datasets (Ye *et al.*, 2013). These catchment characteristics will later be utilized to develop parameterizations of the storage-discharge relationship (i.e., a and b) in terms of landscape soil and topographic properties.

The MOPEX dataset provides daily climate and streamflow data from 438 catchments, covering a wide range of climate conditions, landscapes, and ecosystems, ranging from very humid environments in the Northwest to extremely arid conditions in the Southwest of continental United States: <http://www.nws.noaa.gov/oh/mopex/index.html>. The topographic slope, aridity index and the coefficient and exponent of recession curves were extracted from the MOPEX dataset, while drainage density was extracted from the National Hydrography Dataset (NHD) (<http://nhd.usgs.gov/>) (see also Ye *et al.*, 2013).

Although the MOPEX dataset also provides estimates of saturated hydraulic conductivity, it was a somewhat older qualitative estimate based on soil texture, and the resolution is deemed too coarse for this study. In this study, the soil hydraulic properties are extracted from the USGS SSURGO dataset: <http://soils.usda.gov/survey/geography/ssurgo/>. The SSURGO dataset is provided by the National Resource Conservation Service (NRCS); it includes both spatial data of the measured map unit, and tabular data of the measurements done within each map unit. The resolution of the SSURGO dataset is 30m, which is about 10 times higher than the STATSGO dataset, and is therefore better suited for the detailed analyses performed in this study. The mean and standard deviation of saturated hydraulic conductivity at the surface, the vertical (exponential) decay parameter of the saturated hydraulic conductivity and soil porosity were estimated from this dataset. For this study, the soils data at the catchment scale were extracted in a raster format so as to estimate the first two moments and the standard deviation. A procedure

was developed to merge the SSURGO data, clip the data by the catchment boundary, retrieve the soil porosity (ϕ), which can be used to describe the soil water storage capacity when combined with soil depth (ϕd), saturated hydraulic conductivity at the top and bottom layer as well as the vertically averaged value for each map unit, and then convert the data to raster data type. These reconstructed raster data with the average porosity or saturated hydraulic conductivity at the surface were then used to compute the spatial average hydraulic conductivity value and its standard deviation. Though comprehensive research works have not been carried out to study the exponential decay characteristic of the SSURGO based hydraulic conductivity, several separate research works in the US have been employed to estimate saturated hydraulic conductivity from SSURGO dataset, along with the exponential decay along the soil depth (Kennen et al., 2008; Tesfa, 2010, Nystrom and Burns, 2011). Other similar analyses have been carried out in the Prairies regions of North America by Ireson et al. (2013), Bodhinayake and Cheng Si (2004).

In this paper we will use two of the 50 catchments to demonstrate the up-scaling procedure (as shown in Figure 2). These two catchments were selected because of strong differences in climate, topography and soils. Soquel Creek catchment is located along the Central Coast of California, near the southern end of the Santa Cruz Mountains (Figure 2b – left panel). The catchment covers a drainage area of 104.1 sq. km with two upstream major tributaries. The elevation decreases from 1036 m above sea level at the highest part to 17 m at the river mouth within a distance of only 16 km along the stream. Its climate is Mediterranean with cool, wet winters and hot, dry summers. Council Creek watershed (Figure 2b – right panel) is located in Payne County in north-central Oklahoma. Its drainage area is 80.3 km² and total stream length is 68 km. It belongs to the Southern Great Plains and is relatively flat, with topographic elevation ranging from 333 m at the highest points to 255 m at the river mouth. Table 1 summarizes some of the catchment properties of the catchments and their sources.

In order to set up the hillslope building blocks for the up-scaling, we divide each catchment into a population of sub-catchments organized around its stream network. This is done using an appropriate upstream contributing area threshold that generates a drainage network consistent with the observed blue-line stream network from the NHD dataset. The hillslopes are then defined as land areas draining either side of the stream reach in each sub-catchment and in the case of headwater sub-catchments (area draining into the source node) an additional hillslope to

represent the convergent contributing to a source node. Digital elevation models (DEM) available for all 50 catchments provide the necessary data to partition the catchments into sub-catchments and then into hillslopes. The up-scaling to catchments scale was performed on the basis of hillslope properties extracted for each constituent hillslope such as topographic slope, mean hydraulic conductivity with its spatial variation within the hillslope and hillslope length, whereas other variables such as soil depth and porosity are assumed to be constant.

3. Results and discussion

3.1. Hillslope-scale simulations

As part of the hillslope-scale simulations, sensitivity analyses were used to investigate the impact of topographic slope and saturated hydraulic conductivity of soils, including both their horizontal and vertical variability on saturated storage, for different recharge rates, under steady state conditions. Figure 3 presents an example of the random field of soil saturated hydraulic conductivity generated by the random field model (just one realization). For this we chose a range of values of the landscape properties in a physically meaningful way, guided by field studies.

Figure 4 presents one set of examples of the multiple simulations performed as part of these sensitivity analyses, in each case illustrating the transition from the initial fully saturated condition to the ultimate steady state under the given landscape properties and the assumed recharge rate. Figure 4(a) shows the effect of topographic slope. It can be seen that for the same soil hydraulic properties, an increase in topographic slope leads to pronounced decreases of the steady state storage value. This result, as well as a similar result in response to changes in the surface hydraulic conductivity, is understandable since increase of slope and/or saturated hydraulic conductivity contributes to an increase of the drainage capacity of the hillslope, and a corresponding decrease of water storage. Figure 4(b) presents the corresponding result in respect of the exponential decrease of saturated hydraulic conductivity with depth. Here, the results are presented in terms of f , the product of the decay parameter f , and soil depth d . The results show that water storage in the hillslope decreases with increase of f . Large f means the hydraulic conductivity at the bottom of the soil is small, and which reduces the drainability of the hillslope,

thus helping to retain more water in storage. An opposite result ensues when f is small, and in this way helps to explain the results in Figure 4(b). Figure 4(c) presents the results of sensitivity analyses with respect to the random spatial distribution of hydraulic conductivity. The results show that the impact of the random spatial variability of soil hydraulic conductivity is much less relative to the impacts of the other landscape properties considered in these simulations.

The remainder of the results presented below will utilize the steady state storage values obtained in this way in order to derive the needed storage-discharge relations.

3.2. Developing hillslope scale storage-discharge relations

Multiple hillslope simulations were carried out with the combination of topographic slopes ranging from 5 to 30°, surface hydraulic conductivity K_s ranging from 3 to 42 $\mu\text{m/s}$, f ranging from 0 to 1m^{-1} , $\sigma_{\ln k}^2$ ranging from 0.0 to 2.0, and uniform recharges at the rates q_r ranging from 0.0 to 10mmd^{-1} . In each simulation the same recharge rate was applied over several days until a steady state was reached. Hillslope scale storage-discharge relationships were then derived from the steady state storage recorded in the system and integrated over the entire domain, and the discharges equal to the applied recharge rates. The exponents and coefficients of storage-discharge relationships were obtained by fitting a power-law equation to results of the numerical simulations (using the MATLAB curve fitting tool box).

Figure 5 presents the relationship between landscape properties and the exponent of the storage-discharge relationship curve extracted from the numerical analyses. Figure 5(a) shows the impact of hillslope gradient on the exponent of the S - Q curve, indicating a significant relationship, which can be fitted with a nonlinear relationship ($R_{adj}^2 = 0.56$). The scatter in the result suggests that the exponent also depends on other factors and more than one variable is involved in the most appropriate parameterization, in addition to the topographic slope. Figure 5(b) indicates a nonlinear relationship between the exponent b and surface saturated hydraulic conductivity ($R_{adj}^2 = 0.13$), whereas the linear relationship with f ($R_{adj}^2 = 0.28$) shown in Figure 5(c) appears to be stronger. Exponent b decreases with increase of mean K_s , whereas it increases with increase of the exponential decay parameter, f . Clearly, these two relationships, due to their connection to

the drainability of the hillslope, are inter-related. On the other hand, as seen in Figure 5(d), there appears to be no significant relationship between exponent b and $\sigma_{\ln K}^2$ ($R_{adj}^2 = 0.006$).

Our analysis next involves the selection of the most influential variables to determine the coefficient and the exponent of the hillslope-scale S - Q relationship. The coefficient and exponent must then be expressed in terms of the selected variables in a way that encapsulates the actual processes and accounting for the effects of soil heterogeneity. Stepwise multiple regression analysis yielded the most influential model predictors to form the associated closure relations. The results from possible candidate models from both linear and nonlinear regression analyses shown in Table 2 indicate that topographic slope, surface hydraulic conductivity together with f explain the observed exponents, whereas the impact of random soil heterogeneity, $\sigma_{\ln K}^2$, is found to be negligible. The model predictor based on three selected variables, b ($\tan\theta$, K_s , f) has the least $AICc$ (i.e. -793.2 for linear and -942.4 for nonlinear models) than the full models developed with a combination of all variables. Interestingly, we found that model fits for the reduced model b ($\tan\theta$, K_s , f), i.e., $R_{adj}^2 = 0.918$, is almost as good as for the full model with all parameters included ($R_{adj}^2 = 0.915$). Each of the models in Table 2 was examined based on their performance to predict the observed exponents and the best model was chosen from the regression analyses ranking their influence on the exponent based on the AIC value; the best model turned out to be:

$$b = \frac{\zeta_b \exp(\omega_b f d)}{\tan \theta^\gamma K_s^{\delta_b}} \quad (10)$$

where $\tan\theta$ is the topographic slope, and ζ_b , γ_b , δ_b and ω_b are constants. Figure 6 depicts the good correspondence of the exponent by the proposed model between exponents obtained from numerical simulations and those predicted by the reduced model (Eq. 10).

Using the same approach, the coefficients a of the power-law form of the S - Q relationship were also analyzed in respect of the influence of the same landscape properties. Figure 7 presents how the normalized coefficient $\hat{a} = a(\phi d)^b L^{b-1} / K_s$ changes with topographic slope (Figure 7a), hydraulic conductivity, K_s (Figure 7b), the normalized exponential decay parameter, f (Figure 7c), and the heterogeneity parameter, $\sigma_{\ln K}^2$ (Figure 7d). The results in Figure 7a indicate that the

topographic slope is a poor predictor of a . The result shows very small variation ($\hat{a}$ ranges from 4.98 – 5.29) for constant $K_s = 27.8 \mu\text{ms}^{-1}$, $f = 0.5$ and $\sigma_{\ln k}^2 = 1$ for a large range of the topographic slopes (5° to 30°). On the other hand, K_s and f in Figure 7(b and c) do explain the coefficient well and the variation is within an acceptable range ($R_{adj}^2 = 0.531$ and 0.361). While heterogeneity did not significantly impact b , our result shown in Figure (7d) indicates that $\sigma_{\ln k}^2$ ($R_{adj}^2 = 0.165$) has also impact on a . We found that $\hat{a}$ ranged from 3.7 to 4.6 when $K_s = 14 \mu\text{ms}^{-1}$ and the heterogeneity, $\sigma_{\ln k}^2$ ranged from 0 to 1 with other variables remaining constant.

Based on the analysis from the multiple-regression, variables K_s , f and $\sigma_{\ln k}^2$ were found to be likely the most important controls on the coefficient a . Table 3 presents the performance of some selected regression models, sorted according to their $AICc$ values. Although the R_{adj}^2 for the full (all variable) model is larger than the other models, it is shown that the three-parameter model, a ($K_s, f, \sigma_{\ln k}^2$) has the least $AICc$ (i.e. -211.4 for linear and -464.83 for nonlinear models), indicating that the three variable model can predict the coefficient with minimum inputs. For this reason, this model was chosen and the resulting closure relation for the dimensional form of the coefficient (i.e., denoted as a) is as follows:

$$a = \frac{\zeta_a K_s^{\delta_a + 1} \exp(v_a \sigma_{\ln k}^2 - \omega_a f d)}{(\phi d)^b L^{b-1}} \quad (11)$$

where ζ_a , δ_a , v_a and ω_a are constants, d is the soil depth, ϕ is the porosity and L is the hillslope length. Figure 8 shows a very good comparison between the coefficients predicted by the chosen model (Eq. 11) and the values estimated through numerical simulations.

By combining the expressions for the exponent b and the coefficient a , we can now put together the storage–discharge relationship terms of the total discharge per unit width Q [L^2/T] and total storage per unit width S [L^2] as follows:

$$Q = \frac{\zeta_a K_s^{\delta_a + 1} \exp(v_a \sigma_{\ln k}^2 - \omega_a f d)}{(\phi d)^b L^{b-1}} S^b \quad (12)$$

where b is the exponent estimated from Equation (11), and φ is drainable porosity, and the other variables and constants are as defined before. The constants shown in the equation are presented in Table 4.

Examples of the storage-discharge relationship are presented in Figure 9, generated with synthetic data of the predictor variables. These represent sensitivity analyses with respect to key predictor variables individually, while keeping other predictor variables constant. For example, Figure 9(a) shows that when the topographic slope is increased, with all other variables remaining constant, the exponent of the S - Q curve decreases, whereas the coefficient increases, since it also depends on the exponent. Similarly, Figure 9(b) shows that the exponent of the storage-discharge relationship decreases with increasing saturated hydraulic conductivity and decreasing exponential decay parameter f . On the other hand, the spatial heterogeneity does not have a significant impact on the storage-discharge relationship.

Finally, the disaggregation approach to up-scaling to the catchment scale requires that the storage-discharge relationship given in Equation 12 now be expressed in terms of storage and discharge per hillslope area, and not per unit width of stream. Given that $A_i=L$, defining $q=Q/A_i$ and $s=S/A_i$, we then have the corresponding storage-discharge relationship given as follows:

$$q = \frac{\zeta_a K_s^{\delta_a+1} \exp(\nu_a \sigma_{\ln K}^2 - \varpi_a f d)}{(\varphi d)^b} s^b \quad (13)$$

3.3. Derivation of catchment-scale storage-discharge relationship

The two catchments from the MOPEX dataset were used to demonstrate the up-scaling of the storage-discharge relations from the hillslope to catchment scales. The up-scaling requires sophisticated reprocessing of topographic and soil data. The delineation of sub-catchments and then hillslopes from digital elevation model (DEM) data is built upon a set of techniques developed over the past few years. Figure 10(a) illustrates the delineated hillslopes in the Soquel Creek (left) and Council Creek (right) with accumulation area thresholds of 300 and 200 pixels, respectively, resulting in 431 and 319 hillslopes, respectively. The up-scaling analyses were performed on the basis of the landscape properties extracted for each hillslope (Figure 10 b and c), whereas variables such as soil depth and porosity are assumed constant for all hillslopes.

The up-scaling procedure, i.e., the disaggregation-aggregation approach, outlined in Section 2 is implemented on the two chosen study catchments. We start with representative values of catchment scale discharge, Q , which is converted to uniform recharge $q=Q/A$, assuming steady state condition. Given the value of q , Equation 14 is inverted to generate the magnitudes of the specific storage, $s_i = S_i/A_i$, for all hillslopes within the catchment, using magnitudes of the predictor variables for each component hillslopes and the constants associated with Equations 11 and 12. Due to the lack of detailed information regarding f , we shall determine the S - Q relationship for a range of values of f , rather than use the one estimate we have for each catchment obtained from the limited information available. This is done to assess the importance of the f parameter and to provide some insight into the uncertainty of the model predictions.

Results presented in Figure 11 shows the storage, s [L] – discharge, q [LT^{-1}] relationships of the Soquel Creek and Council Creek catchments, aggregated from the hillslope scale, for a range of values of the f parameter. It can be seen that the S - Q relationships derived through up-scaling match the results obtained from analysis of recession curves (Ye *et al.*, 2013) for $f \approx 0.4m^{-1}$ at the Soquel Creek and $f \approx 0.3m^{-1}$ at Council Creek. The results also indicate considerable sensitivity of the resulting storage-discharge relationships to the magnitude of the f parameter. It can be seen that Soquel Creek exhibits strong nonlinearity in the s - q relationship ($b = 1.35$) whereas Council Creek is more linear ($b = 0.98$). The non-linearity is influenced by topographic slope, and also the magnitude of the surface hydraulic conductivity in Soquel Creek. Also, subsurface flow at Soquel Creek originates in the upper catchment, which has a large contribution to the stream, and less water is stored due to the change of relief and high surface hydraulic conductivity (Figure 10). Conversely, in Council Creek, topography is relatively flat, and much of the infiltrated water is stored in the subsurface, and therefore subsurface discharge is relatively low.

3.4. Regionalization of storage-discharge relationship across MOPEX catchments

The up-scaling analyses presented in Section 3.3 above were repeated, and storage-discharge relationships and associated coefficients a and exponents b were derived for all 50 catchments, once again for a range of values of the parameter f . In order to be able to compare these against empirical results obtained through analysis of observed streamflow recession curves, the parameters a and b are converted to parameters α and β associated with the recession slope

curves (Equations 2 and 3). Multiple regression analyses were next performed against the combination of predictor variables identified as predictors, with the best models selected as those having the lowest AICc value. The resulting expressions for α and β are given below:

$$\alpha = \frac{0.0104\theta^{0.67}K_s^{0.92}D_p^{0.01}}{(\phi d)^{0.37}} e^{-(0.85\sigma_{\ln k} + 0.31f)} \quad (14)$$

$$\beta = 1.297(\phi d)^{0.1} e^{0.15f - 0.01\theta} \quad (15)$$

The result from the theoretical up-scaling approach indicates that the coefficient α of recession curves is a function of topographic slope, surface saturated hydraulic conductivity, porosity, soil depth, and drainage density (i.e. consists of the river network length and the drainage area), which is consistent with the results of previous theoretical studies (Brutsaert and Lopez, 1998, Harman and Sivapalan, 2009a). Similarly, the result that the exponent depends on soil depth and the exponential decay parameter, f , is also consistent with previous theoretical studies (Rupp and Selker, 2005, 2006). The main difference of the present study is that it incorporates the effects of spatial variability of both soil properties and topographic slope, whereas previous results only apply at the hillslope scale with uniform properties.

Now, by fixing the values of the parameter, f , to the estimate obtained from the SSURGO soil dataset for each of the 50 MOPEX catchments (Ye *et al.*, 2013), regional variations of the magnitudes of α and β can be generated. These are presented in Figure 12 (a) and (b). It is seen that α is small in the south-eastern part of USA where lowlands are the dominant topographic feature, whereas α values are higher in the northeast and in catchments in the south-central part. On the other hand, high values of β are found in the east and relatively low values in the center. Figure 12 (c) and (d) present the corresponding results derived empirically from the recession curves (taken from Ye *et al.*, 2013). They show that there are substantial deviations between the theoretical results and those obtained from the observed recession curves, and that the theoretically derived α and β show no apparent relationship to the empirical values derived from recession curve analysis. Admittedly, this is a negative outcome of the up-scaling approach. This could be attributed to: (1) the small scale model, which in this case is based on the Richards equation, and its appropriateness in the context of the real world systems, (2) small scale soil

parameters, and their representativeness, (3) the up-scaling method, including the assumptions made, such as the steady state assumption, and the assumption of complete continuity of the subsurface system all the way to the top of the hillslope. For example, the Richards equation formulation is unable to directly account for the effects of macropore flow and other heterogeneities, and only indirectly through the exponential decay with depth of hydraulic conductivity. Even if we had a model that can account for these effects, there is the added problem of obtaining the corresponding parameter values in the chosen actual catchments from standard data. In any case this raises real questions about developing these parameterizations in the short term using the bottom-up approach alone.

In spite of this negative result, further insights into the deviations can be obtained by computing the ratios of the theoretical estimates against the empirical (true) estimates obtained by Ye *et al.* (2013). Again, guided by observations of Ye *et al.* (2013), we look for a dependence of these ratios upon the climatic aridity index (E_p/P , ratio of annual potential evaporation over annual precipitation). Figure 13 presents scatter plots of the ratios (theoretical over the empirical/true) of the coefficients, α , and exponents, β . It shows that the ratio of the exponents, β , shows a clear dependence on E_p/P , providing an interesting insight into the discrepancies between the empirical and theoretical results, whereas the ratio of α values does not show any dependence on E_p/P . The dependence on climate is by far the most important result here. Given that the theoretically derived exponent β has no climate dependence, this is due to the fact that the empirically derived β decreases with increasing aridity E_p/P (from Ye *et al.*, 2014). In view of the direct relationship (both theoretical, see Equation 15, and empirical – see Ye *et al.*, 2014) between β and the exponential decrease parameter f , the climate dependence of β implies a climate dependence of f (for which some evidence exists in Ye *et al.*). Especially, this further implies that the more arid a catchment is, the smaller f is (which means a deeper hydrologically active layer, deeper root zone, or deep roots): this is a sequence of associations that remain to be further explored in an eco-hydrological and hydro-pedological sense.

The deviations between the theoretically and empirically derived values of the recession-slope curve parameters can be attributed to several factors: 1) the dependence on climate as discussed above; 2) the inappropriateness of the Darcy's Law-based Richards equation model to account for the structure of heterogeneity present within a catchment; and 3) the uncertainty in the

estimates of both topographic and soil hydraulic properties, e.g., estimates of soil heterogeneity and the vertical delay parameter. Besides the disparity of the magnitudes of the parameters obtained by the two approaches which may be attributed to the factors already discussed, the parameterizations obtained have nevertheless shown that the subsurface flow can be described by similar landscape characteristics and soil properties in both approaches (this paper and that of Ye et al., 2014). The theoretical approach is superior because of its physical basis and the fact the results can be interpreted physically as compared to the existing techniques. In fact, it was carried out using rigorous procedures to develop a single parameterization of subsurface flow through upscaling from point to hillslope scale and then from hillslope to catchment scale. The parameterization we obtained at the catchment scale can be used for any catchment without doing any numerical simulations at the hillslope scale which makes this approach more easy and simple to implement. Improvements to address the weaknesses, including fundamental research to understand the co-dependence of soil and topographic properties, can contribute towards improved estimates of the recession curve parameters (and storage-discharge relationships) in ungauged locations.

4. Conclusions

The main aim of this study has been the development of physically based storage-discharge relations governing subsurface stormflow at the catchment scale through parameterization of the effects of within-catchment landscape heterogeneity (i.e., heterogeneity of soil hydraulic properties and key topographic features). The approach involved a two-stage up-scaling. In the first stage, storage-discharge relations were derived at the hillslope scale, accounting for random and systematic heterogeneity of soil hydraulic properties, through recourse to Monte Carlo simulations with a 3-D distributed saturated-unsaturated numerical model of Richards' equation on idealized hillslopes with synthetically generated soil properties. On the basis of the simulation results regression relationships were derived between the parameters of a power-law form of the storage-discharge relationships (namely the coefficient a , and exponent b) and measureable soil and topographic properties at hillslope scale. In the second stage, a separate up-scaling procedure was adopted that enabled the effects of the heterogeneity of topographic slopes and hillslope lengths present within actual catchments, leading to new regressions that connected catchment

scale parameters a and b to catchment scale soil and topographic properties. The results obtained are consistent with previous theoretical studies at the hillslope and catchment scales.

The up-scaling procedure was implemented in 50 catchments in eastern United States, and the resulting storage-discharge relations were compared to relationships obtained through regionalization of storage-discharge relations derived from empirical streamflow recession curves. This brought out considerable disparity between the results from these two alternative bottom-up (this study) and top-down (parallel study of Ye *et al.*, 2013) approaches. While both approaches led to functional forms for a and b that were similar, the actual magnitudes of a and b were quite different.

Comparison with observed exponents showed that in real catchments there is a climate dependence of the storage-discharge relationships, which current physical theory is not able to accommodate. This problem has been recognized in current application of LSMs, and is indeed accommodated through building in a dependence of the model parameters on climate (see e.g., Nijssen *et al.*, 2001; Xie *et al.*, 2007). For the immediate purpose of developing improved, physically based parameterizations of subsurface flow for LSMs, the way forward then is to bring about a synthesis of the bottom-up (this paper) and top-down approaches (Ye *et al.*, 2014). This will introduce a physical basis into the empirical parameterizations, while grounding the theoretical relationships with empirical observations. This will be the next step in this line of research.

In the long-term, however, this raises fundamental questions regarding possible ways forward: (i) how representative are the field measured point-scale soil hydraulic properties, even after accounting for random spatial heterogeneity, of hillslope and catchment scale subsurface flow processes? (ii) how do we account for natural organization of the soil properties over and above the random heterogeneity, including the presence of macropores (Beven and Germann, 2013) and flow discontinuity and partial saturation, which are issues that have been brought out in many field studies? and (iii) how do we account for the co-dependence of climate, soils, topography and vegetation in numerical models of subsurface flow. These are questions that are raised through the work done in this paper, and answers to these questions will require new and fundamental research, which is beyond the scope of this paper. Clearly, a synthesis of the

bottom-up and top-down approaches followed in this work and that of Ye et al. (2014) is needed, which is the next line of research in this direction.

Appendix A

Mathematical framework and numerical Modeling

We simplify the hillslope as a sloped parallelepiped and use a dimensionless formulation of shallow subsurface flow based on a 3-D Richards' equation developed by Ali et al (2013). The hillslope is characterized as a heterogeneous planar, rectangular hillslope of 100 m length, 20 m width and 5 m depth, with a constant topographic slope. In this study we choose the dimensions such that we can neglect runoff caused by the emergence of a water table over the ground level. The form of the Richards' equation used is given by:

$$C(h) \frac{\partial h}{\partial t} = \nabla \cdot \{k(h) \nabla (h + z)\} \quad (\text{A1})$$

where $C(h)=\partial\theta/\partial h$ represents the specific moisture content [L^{-1}], t is the time [T], h is the pressure head [L], z are the elevation head [L], and $K(h)$ is the hydraulic conductivity [$L T^{-1}$]

It is assumed that the local effective degree of saturation and unsaturated hydraulic conductivity are described by the Brooks and Corey (1964) functional relationship; i.e. $S_e = (\theta - \theta_r)/(\varphi - \theta_r) = (h_b/h)^\lambda$, where S_e is the effective saturation, θ_r is the residual volumetric water content, φ is the porosity, h_b is the bubbling or air entry pressure head, and λ is the pore size distribution index. The specific moisture content $C(h)$ therefore becomes

$$C(h) = \frac{\partial \theta}{\partial h} = -\lambda(\varphi - \theta_r) \left(\frac{h_b^\lambda}{h^{\lambda+1}} \right) \quad (\text{A2})$$

The hydraulic conductivity is defined as a function of the saturated hydraulic conductivity (K_s), the bubbling pressure (h_b), the pressure head (h) and the pore size index λ ($n=3+2/\lambda$) as follows:

$$K(h) = K \left(\frac{h_b}{h} \right)^{n\lambda} \quad (\text{A3})$$

A dimensionless form of the Richards equation is derived by normalizing the specific moisture content, the volumetric water content, the pressure head, the hydraulic conductivity of the material and the sink/source term using the appropriate scaling variables. We adopt dimensionless variables by rescaling their dimensional values by the hillslope length L , soil depth d and mean surface hydraulic conductivity K_m . The resulting non-dimensional variables are: $\hat{x} = x/L$, $\hat{y} = y/L$, $\hat{z} = z/d$, $\hat{h} = h/d$, $\hat{h}_b = h_b/d$, $\hat{t} = tK / L(\phi - \theta_r)$ and $\hat{K}_s = K_s / K_m$ where x , y and z are the spatial coordinates.

The dimensionless form of Richards' equation is solved by the finite element method using the earth science module of Comsol Multiphysics software that employs numerical methods to solve partial differential equation (COMSOL AB, 2010). The output variables from the model that are of interest are also dimensionless (interested readers are referred to Ali *et al.*, 2012 for details of the dimensional analyses).

In these simulations, the initial condition is one where the water table is at the surface and the system is fully saturated. The boundary condition at the upper boundary is an assumed net precipitation, which is assumed normal to the hillslope. The bottom boundary is a no-flow boundary; the same is true for the right, left and upper vertical planes parallel and normal to the flow direction. A seepage face is assumed at the right boundary where water discharges from the domain. The boundary face is divided into a Dirichlet boundary condition for the seepage face (along which the prescribed internal pressure $p = 0$) and the Neumann condition for the region above the seepage face Chui and Freyberg (2007). The temporal variability of the size of the seepage face is automatically accounted for by the method. At the end of the simulation, when steady state conditions establish, the total water content in the hillslope is recorded and employed in the recession analysis of Section 3.2.

Acknowledgements

This study was supported by the Office of Science of the U.S. Department of Energy as part of the IMPACTS project funded by the Earth System Modeling program to improve hydrologic

parameterizations in land surface models for predicting changes in droughts in the future climate. PNNL is operated for DOE by Battelle Memorial Institute under Contract DE-AC05-76RLO1830.

5. References

- Akaike, H. (1974), A new look at the statistical model identification. *IEEE Transactions on Automatic Control*, 19 (6): 716–723, doi:10.1109/TAC.1974.1100705, MR 0423716.
- Ali, M., Fiori, A. and Bellotti, G. (2013), Analysis of the nonlinear storage–discharge relation for hillslopes through 2D numerical modelling. *Hydrol. Process.*, 27: 2683–2690. doi: 10.1002/hyp.9397
- Bachmair, S., and M. Weiler (2012), Hillslope characteristics as controls of subsurface flow variability, *Hydrol. Earth Syst. Sci.*, 16, 3699–3715, doi:10.5194/hess-16-3699-2012.
- Bellin, A., and Y. Rubin (1996), HYDRO_GEN: A spatially distributed random field generator for correlated properties. *Stoch. Hydrol. and Hydraul.*, 10, 253–278.
- Beven, K. J., and M. J. Kirkby (1979), A physically based, variable contributing area model of basin hydrology, *Hydrol. Sci. Bull.*, 24, 43–69.
- Beven, K. J. (1982). On subsurface stormflow: an analysis of response times. *Hydrol. Sci. J.*, 27(4): 505–521.
- Beven, K., and P. Germann (2013), Macropores and water flow in soils revisited, *Water Resour. Res.*, 49, 3071–3092, doi:10.1002/wrcr.20156
- Bogaart, P. W., and P. A. Troch (2006), Curvature distribution within hillslopes and catchments and its effect on the hydrological response, *Hydrol. Earth Syst. Sci.*, 10, 925–936, doi:10.5194/hess-10-925-2006.
- Brooks R. J., and Corey A. T. (1964), Hydraulic properties of porous media, *Hydrol. Pap.* 3, Colo. State Univ., Fort Collins.
- Brutsaert, W., and J. L. Nieber (1977), Regionalized drought flow hydrographs from a mature glaciated plateau. *Water Resour. Res.*, 13, 637–643, doi: 10.1029/WR013i003p00637.
- Brutsaert, W., and J. P. Lopez (1998), Basin-scale geohydrologic drought flow features of riparian aquifers in the southern Great Plains. *Water Resour. Res.*, 34 (2), 233–240.
- Chui, T., and D. Freyberg (2007). The Use of COMSOL for Integrated Hydrological Modeling. COMSOL Conference, Boston, MA, COMSOL, Inc., 217–223.

772 COMSOL AB (2010), COMSOL Multiphysics Earth Science Module User's Guide (Version
773 4.0a).

774 Duffy, C. J. (1996), A two-state integral-balance model for soil moisture and groundwater
775 dynamics in complex terrain. *Water Resour. Res.*, 32(8), 2421-2434.

776 Duan Q., J. Schaake, V. Andreassian, S. W. Franks, H. V. Gupta, Y. M. Gusev, F. Habets, A.
777 Hall, L. Hay, T. Hogue, M. Huang, G. Leavesley, X. Liang, O. N. Nasonova, J. Noilhan, L.
778 Oudin, S. Sorooshian, T. Wagener, and E. F. Wood (2006), Model Parameter Estimation
779 Experiment (MOPEX): Overview and Summary of the Second and Third Workshop Results.
780 *J. Hydrol.*, 320, 3-17, doi:10.1016/j.jhydrol.2005.07.031.

781 El-Kadi, A., and W. Brutsaert (1985), Applicability of effective parameters for unsteady flow in
782 nonuniform aquifers. *Water Resour. Res.*, 21(2), 183-198.

783 Fiori, A. (2012). Old water contribution to streamflow: Insight from a linear Boussinesq model.
784 *Water Resour. Res.*, 48(6), W06601.

785 Fiori, A., and D. Russo (2007), Numerical analyses of subsurface flow in a steep hillslope under
786 rainfall: The role of the spatial heterogeneity of the formation hydraulic properties. *Water*
787 *Resour. Res.*, 43, W07445, doi:10.1029/2006WR005365.

788 Freer J., J. J. McDonnell, K. J. Beven, D. Brammer, D. Burns, R. P. Hooper, and C. Kendall
789 (1997), Topographic controls on subsurface storm flow at the hillslope scale for two
790 hydrologically distinct small catchments. *Hydrol. Process.*, 11, 1347–1352.

791 Fujimoto, M., N. Ohte, and M. Tani (2008), Effects of hillslope topography on hydrological
792 responses in a weathered granite mountain, Japan: comparison of the runoff response
793 between the valley-head and the side slope. *Hydrol. Process.*, 22, 2581–2594.

794 Harman, C., and M. Sivapalan (2009a), A similarity framework to assess controls on shallow
795 subsurface flow dynamics in hillslopes, *Water Resour. Res.*, 45, W01417,
796 doi:10.1029/2008WR007067.

797 Gardner, W. R. (1958). Some steady-state solutions of unsaturated moisture flow equations with
798 application to evaporation from a water table. *Soil Science*, 85, 228–232.

799

800 Harman, C. J., and M. Sivapalan (2009b), Effects of hydraulic conductivity variability on
801 hillslope-scale shallow subsurface flow response and storage-discharge relations. *Water*
802 *Resour. Res.*, 45, W01421, doi:10.1029/2008WR007228.

- Hou, Z., M. Huang, L. R. Leung, G. Lin, and D. M. Ricciuto (2012), Sensitivity of surface flux simulations to hydrologic parameters based on an uncertainty quantification framework applied to the Community Land Model, *J. Geophys. Res.*, 117, D15108, doi:10.1029/2012jd017521.
- Huang, M., and X. Liang (2006), On the assessment of impact of reducing parameters and identification of parameter uncertainties in the VIC-3L model with applications to ungauged basins. *J. Hydrol.*, 320, 37–61, doi:10.1016/j.jhydrol.2005.07.010.
- Huang, M., X. Liang, and L. R. Leung. (2008). A generalized subsurface flow parameterization considering subgrid spatial variability of recharge and topography. *J. Hydrometeorol.*, 9, 1151–1171. doi: <http://dx.doi.org/10.1175/2008JHM936.1>
- Huang, M., Z. Hou, L. R. Leung, Y. Ke, Y. Liu, Z. Fang, and Y. Sun (2013), Uncertainty analysis of runoff simulations and parameter Identifiability in the Community Land Model - Evidence from MOPEX Basins, *J. Hydrometeorol.*, doi:10.1175/JHM-D-12-0138.1.
- Ireson, A.M., G. van der Kamp, U. Nachshon, A. P. Butler (2013). Modeling groundwater-soil-plant-atmosphere exchanges in fractured porous media, *Procedia Environmental Sciences*, 19, 321-330, ISSN 1878-0296, <http://dx.doi.org/10.1016/j.proenv.2013.06.037>.
- Kennen J.G., L. J. Kauffman, M. A. Ayers and D. M. Wolock (2008) Use of an integrated flow model to estimate ecologically relevant hydrologic characteristics at stream bio-monitoring sites. *Ecological Modelling*, 211, 57–76.
- Lee H., M. Sivapalan, and E. Zehe (2005), Representative Elementary Watershed (REW) approach, a new blueprint for distributed hydrologic modelling at the catchment scale: the development of closure relations. In: *Predicting Ungauged Streamflow in the Mackenzie River Basin: Today's Techniques & Tomorrow's Solutions*, C. Spence, J. W. Pomeroy and A. Pietroniro (Editors), Canadian Water Resources Association (CWRA), Ottawa, Canada.
- Liang, X., D. P. Lettenmaier, E. F. Wood, and S. J. Burges. (1994), A simple hydrologically based model of land surface water and energy fluxes for general circulation models. *J. Geophys. Res.*, 99(D7), 14, 415–14.
- Liang, X., D. P. Lettenmaier, and E. F. Wood (1996), One dimensional statistical dynamic representation of subgrid spatial variability of precipitation in the two-layer variable infiltration capacity model. *J. Geophys. Res.*, 101(D16), 21403–21422.

833 McDonnell, J. J. (1990). A rationale for old water discharge through macropores in a steep,
834 humid catchment. *Water Resour. Res.*, 26(11), 2821-2832.

835 Nijssen, B., G.M. O'Donnell, D. P. Lettenmaier, D. Lohmann and E.F. Wood (2001). Predicting
836 the discharge of global rivers. *J. Climate*, 14, 3307–3323.

837 Niu, G.-Y., Z.-L. Yang, R. E. Dickinson, and L. E. Gulden (2005), A simple TOPMODEL-based
838 runoff parameterization (SIMTOP) for use in global climate models, *J. Geophys. Res.*,
839 110(D21), D21106, DOI: 10.1029/2005JD006111.

840 Niu, G.-Y., Z.-L. Yang, R. E. Dickinson, L. E. Gulden, and H. Su (2007), Development of a
841 simple groundwater model for use in climate models and evaluation with Gravity Recovery
842 and Climate Experiment data, *J. Geophys. Res.*, 112(D7), D07103,
843 DOI: 10.1029/2006JD007522.

844 Nystrom E.A. and D. A. Burns (2011). TOPMODEL simulations of streamflow and depth to water table
845 in Fishing Brook Watershed. U.S. Department of the Interior, U.S. Geological Survey New
846 York O'Loughlin, E. M. (1981). Saturation regions in catchments and their relations to soil
847 and topographic properties. *J. Hydrol.*, 53, 229-246.

848 Parlange, J-Y, and W. Brutsaert (1987). A capillarity correction for free surface flow of
849 groundwater. *Water Resour. Res.*, 23(5), 805–808.

850 Robinson, J. S., and M. Sivapalan (1995), Catchment-scale runoff generation model by
851 aggregation and similarity analyses. *Hydrol. Process.*, 9(5-6), 555-574.

852 Rupp, D. E., and J. S. Selker (2005), Drainage of a horizontal Boussinesq aquifer with a power
853 law hydraulic conductivity profile. *Water Resour. Res.*, 41, W11422.
854 DOI:10.1029/2005WR004241.

855 Rupp, D. E., and J. S. Selker. (2006), On the use of the Boussinesq equation for interpreting
856 recession hydrographs from sloping aquifers. *Water Resour. Res.*, 42(12), W12421,
857 doi:10.1029/2006WR005080.

858 Seibert, J., K. Bishop, A. Rodhe A and J. J. McDonnell (2003). Groundwater dynamics along a
859 hillslope: A test of the steady state hypothesis. *Water Resour. Res.*, 39, 1014,
860 DOI:10.1029/2002WR001404.

861 Sidle, R.C., Y. Tsuboyama, S. Noguchi, I. Hosoda, H. Fujieda, and T. Shimizu (2000).
862 Stormflow generation in steep forested headwaters: a linked hydrogeomorphic paradigm.
863 *Hydrol. Process.*, 14(3), 369–385.

- Sivapalan, M., K. Beven and E. F. Wood (1987), On hydrologic similarity: 2. A scaled model of storm runoff production. *Water Resour. Res.*, 23(12), 2266-2278.
- Sivapalan, M. (1993). Linking hydrologic parameterisations across a range of scales: hillslope to catchment to region. In: Bolle, H.-J., R. A. Feddes and J. D. Kalma (Eds), *Exchange Processes at the Land Surface for a Range of Space and Time Scales*, IAHS Publ., 212, 115-123.
- Sloan, W. (2000). A physics-based function for modeling transient groundwater discharge at the watershed scale. *Water Resour. Res.*, 36(1), 225–241. DOI:10.1029/1999WR900221.
- Sugiura, N. (1978), Further analysis of the data by Akaike's information criterion and the finite corrections. *Commun. Stat. Theory & Methods*, A7, 13–26.
- Todini, E. (1996), The ARNO rainfall-runoff model. *J. Hydrol.*, 175, 339–382.
- Troch, P.A., E. E. van Loon, and A. Hilberts (2002). Analytical solutions to a hillslope-storage kinematic wave equation for subsurface flow, *Adv. in Water Resour.*, 25(6), 727-739.
- Troch, P. A., C. Paniconi, and E. van Loon (2003), Hillslope-storage Boussinesq model for subsurface flow and variable source areas along complex hillslopes: 1. Formulation and characteristic response. *Water Resour. Res.*, 39, 1316, doi:10.1029/2002WR001728.
- Viney, N. R., and M. Sivapalan (2004). A framework for scaling of hydrologic conceptualizations based on a disaggregation–aggregation approach. *Hydrol. Process.*, 18, 1395–1408. doi: 10.1002/hyp.1419
- Xie, Z. H., F. Yuan, Q. Y. Duan, J. Zheng, M. L. Liang and F. Chen (2007). Regional parameter estimation of the VIC land surface model: Methodology and application to river basin in China. *J. Hydrometeorol.*, 8, 447–468. DOI:10.1175/JHM568.
- Ye, Sheng, H.-Y Li, M-Y Huang, M. Ali, G. Leng, L.R. Leung , S.-W. Wang and M. Sivapalan (2013). Regionalization of Subsurface Stormflow Parameters of Hydrologic Models: Derivation from Regional Analysis of Streamflow Recession Curves. Submitted to *J. Hydrol.* (this issue).
- Yeh, P. J.-F., and E. A. B. Eltahir (2005), Representation of water table dynamics in a land-surface scheme. Part I: Model development. *J. Climate*, 18, 1861–1880.

892 Table 1: Summary of the available and source of data for the study areas

Data description	Soquel Creek	Council Creek	Data source
Area (km ²)	104.1	80.3	DEM (US geological survey)
Max./min/ Elevation (m)	1038/17	362/263	
Mean K _s (μms ⁻¹)	43.04	17.3	Soil survey Geographic (SSURGO)
Depth to bed rock (m)	0.89	1.21	Miller and White, 1998
Recession parameter			Ye et al. (2013)
α (mm ^{1-β} /day ^{2-β})	1.26	1.97	and the flow data from MOPEX dataset
β	2.16	0.99	

893

894

895

896

897

898

899

900

901

902

903

904

905

Table 2: Model results from some selected subsets of variables estimating the exponent, b , ranked based on their AICc value from the nonlinear regression models

Model	Linear		Non linear	
	AICc	Radj ²	AICc	Radj ²
$b(\tan \theta, K_s, f)$	-793.206	0.86	-942.339	0.9156
$b(\tan \theta, K_s, f, \sigma_{\ln k}^2)$	-834.163	0.8616	-938.296	0.9181
$b(\tan \theta, f)$	-752.149	0.7789	-813.021	0.8389
$b(\tan \theta, K_s)$	-605.053	0.5389	-639.537	0.5928
$b(\tan \theta, K_s, \sigma_{\ln k}^2)$	-601.628	0.5396	-639.376	0.5947
$b(K_s, f)$	-540.144	0.334	-553.714	0.3523
$b(K_s, \sigma_{\ln k}^2)$	-476.018	0.1304	-140.111	0.1353

Table 3: Model results from some selected subsets of variables estimating the coefficient, a , ranked based on their AICc value from the nonlinear regression models

Model	Linear		Non linear	
	AICc	Radj ²	AICc	Radj ²
$a(K_s, f, \sigma_{\ln k}^2)$	-211.412	0.913	-464.837	0.984
$a(\tan \theta, K_s, f, \sigma_{\ln k}^2)$	-143.924	0.912	-461.139	0.985
$a(K_s, f)$	-47.1981	0.784	-98.456	0.896
$a(\tan \theta, K_s, f)$	-45.2088	0.782	-97.6005	0.896
$a(K_s, \sigma_{\ln k}^2)$	111.5569	0.488	117.0458	0.620
$a(\tan \theta, K_s, \sigma_{\ln k}^2)$	113.3526	0.485	118.3311	0.619
$a(\tan \theta, K_s)$	154.0044	0.355	159.4687	0.527

932

933 Table 4: Regression constants present in the closure equations

Constants	Coefficient	Exponent
ζ	0.65	0.92
δ	0.73	0.11
ω	0.17	0.07
ν	0.21	-
γ	-	0.26

934

935

936

937

938

939

940

941

942

943

944

945

946

947

948

949

950

951

952

953

954 Figure 1: Representation of real hillslope with the hypothetical hillslope modeling. The hillslopes
 955 are defined as land areas draining either side of the stream reach in each sub-catchment and in
 956 the case of headwater sub-catchments (area draining into the source node) an additional hillslope
 957 to represent the convergent contributing to a source node. The natural hillslopes are assumed
 958 rectangular with hillslope length L along the flow path to the channel.

959

Figure 2. (a) Location of MOPEX catchments

Figure 2b: Elevation map with river network of a) Soquel Creek watershed, CA b) Council Creek watershed, OK

969

970

971

972 **Figure 3:** Example of plan view and cross-sectional view of hydraulic conductivities [$\ln K$] are
 973 shown. (K_s - Mean surface hydraulic conductivity of $14\mu\text{ms}^{-1}$ and $\sigma^2=0.5$). The flow
 974 domain, which represents a hillslope flow system, is three dimensional (3D) and
 975 spans 5m depth, 20m width and 100m length along the Cartesian coordinate system
 976 (XYZ) where Z is directed vertically downward. The cross-sectional view across the
 977 X-axis at 10 m in order to provide a view inside the slope with varying K along the
 978 soil depth ($f = 1\text{m}^{-1}$)

979

980

981

982

Figure 4 : Sensitivity analysis of the saturated storage for a) the topographic slope θ , assuming heterogeneous surface soil of $\sigma^2 = 1$, $f = 0$, and constant recharge $q_r = 5\text{mmd}^{-1}$ b) exponential decay parameter f assuming heterogeneous surface soil of $\sigma^2 = 1$, topographic slope of $\theta = 10^\circ$, and constant recharge of $q_r = 10\text{mmd}^{-1}$ c) the spatial variability of the surface soil hydraulic conductivity, assuming slope $\theta = 10^\circ$, $f = 0$, and constant recharge of $q_r = 10\text{mmd}^{-1}$

995

996

997 Figure 5: The exponent of the power law storage – discharge relationship curve plotted against a)
 998 topographic slope b) Surface hydraulic conductivity c) exponential decay parameter,
 999 and d) surface heterogeneity of the hydraulic conductivity

1000

1001

1002

1003

1004

1005

Figure 6: The exponent of the power law storage – discharge relationship curve derived from numerical dataset plotted against the predicted value computed from equation (10)

Figure 7: The normalized coefficient of the power law storage – discharge relationship curve plotted against a) topographic slope b) Surface hydraulic conductivity c) exponential decay parameter, and d) surface heterogeneity of hydraulic conductivity

Figure 8: The coefficient of the power law storage – discharge relationship curve derived from the numerical dataset plotted against the predicted value computed from equation (11)

Figure 9 : Storage – discharge relationship derived from the closure equations for synthetic data with variable a) topographic slope ranges 0 to 30° with 5° interval (other variables are $K_s = 14 \mu\text{ms}^{-1}$, $f = 1 \text{m}^{-1}$ and $\sigma_{\ln K_s}^2 = 1$) b) Hydraulic conductivity K_s ranging from $5 \mu\text{ms}^{-1}$ to $40 \mu\text{ms}^{-1}$ with $5 \mu\text{ms}^{-1}$ interval ($f = 1 \text{m}^{-1}$, $\theta = 10^\circ$ and $\sigma_{\ln K_s}^2 = 1$) c) f ranging from 0 to 2m^{-1} with 0.25m^{-1} interval ($K_s = 14 \mu\text{ms}^{-1}$, $\theta = 10^\circ$ and $\sigma_{\ln K_s}^2 = 1$) and d) $\sigma_{\ln K_s}^2$ ranging from 0 to 2 with 0.25 interval ($K_s = 14 \mu\text{ms}^{-1}$, $\theta = 10^\circ$ and $f = 1 \text{m}^{-1}$)

Figure 10 : a) Hillslope delineation of Soquel Creek watershed (left : accumulation area threshold of 300) and Council Creek watershed (right: accumulation area threshold of 200) b) Hillslope average topographic slope c) Hillslope average surface hydraulic conductivity of Soquel Creek watershed (left) and Council Creek watershed (right)

Figure 11 : Storage discharge curve derived from the hillslope modelling for several values of f ranges from 0 to 1m^{-1} with 0.1m^{-1} interval (solid lines) and recession analysis of observed stream flow (dot) a) Soquel Creek b) Council Creek

1057 Figure 1 : Spatial distribution of the recession curve parameters a) α b) β c) the scattered plot of
1058 theoretical versus empirical α values and d) the same as c but for β .

1060

1061

1062 Figure 2 : Scatter plots of the ratios (theoretical over the empirical/true) of the coefficients, α ,
1063 and exponents, β .