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Infiltration from the pedon to global grid scales: An overview and outlook for land surface modelling

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53 Core ideas:

- 54 Land surface models (LSM) show a large variety in describing and upscaling infiltration
- 55 Soil structural effects on infiltration in LSM are mostly neglected
- 56 New soil databases may help to parametrize infiltration processes in LSM

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Keywords: land surface models, infiltration, soil structure, upscaling, soil databases 58

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109 Abstract

110 Infiltration in soils is a key process that partitions precipitation at the land surface in surface runoff and 111 water that enters the soil profile. We reviewed the basic principles of water infiltration in soils and we 112 analyzed approaches commonly used in Land Surface Models (LSMs) to quantify infiltration as well as its 113 numerical implementation and sensitivity to model parameters. We reviewed methods to upscale 114 infiltration from the point to the field, hill slope, and grid cell scale of LSMs. Despite the progress that has 115 been made, upscaling of local scale infiltration processes to the grid scale used in LSMs is still far from 116 being treated rigorously. We still lack a consistent theoretical framework to predict effective fluxes and 117 parameters that control infiltration in LSMs. Our analysis shows, that there is a large variety in approaches 118 used to estimate soil hydraulic properties. Novel, highly resolved soil information at higher resolutions 119 than the grid scale of LSMs may help in better quantifying subgrid variability of key infiltration parameters. 120 Currently, only a few land surface models consider the impact of soil structure on soil hydraulic properties. 121 Finally, we identified several processes not yet considered in LSMs that are known to strongly influence 122 infiltration. Especially, the impact of soil structure on infiltration requires further research. In order to 123 tackle the above challenges and integrate current knowledge on soil processes affecting infiltration 124 processes on land surface models, we advocate a stronger exchange and scientific interaction between 125 the soil and the land surface modelling communities.

126

128 **1. General Introduction**

129 Infiltration or water entry into the soil profile is a key process in the hydrological cycle. Its rate and 130 dynamics affect the partitioning of precipitation at the land surface and determines the onset of ponding 131 and consequently, the formation of overland flow and runoff. Infiltration affects irrigation efficiency over 132 managed lands and the resulting stored soil water available to vegetation (e.g., Verhoef and Egea-Cegarra, 133 2013), overland flow and soil erosion processes (e.g., Assouline and Ben-Hur, 2006, Garrote and Bras, 134 1995, Poesen et al., 2003), groundwater recharge (e.g., Dahan et al., 2008), the exchange of water and 135 energy between the soil and atmosphere by controlling soil water content at the surface (Kim et al., 2017, 136 MacDonald et al., 2017), and with this the flux partitioning into latent and sensible heat flux with multiple 137 atmospheric feedbacks (e.g., Keune et al., 2016, Seneviratne et al., 2010), stream flow and flooding events 138 (Garrote and Bras, 1995), and various soil physical processes such as the onset of landslides (Lehmann and 139 Or, 2012) and soil mechanical stress-strain behavior. The spatial distribution of infiltration rates is affected 140 by soil type, local topography and attributes of surface cover. Infiltration feedbacks have been shown to 141 drive the formation of vegetation patterns. Infiltration rates are crucial inputs to design any irrigation 142 system and many soil and water conservation practices. The significance of infiltration made it a subject 143 of studies in many domains ranging from hydrology, agricultural, environmental and civil engineering.

144 Even at the single profile scale, infiltration exhibits strong dynamics that are dependent on soil properties, 145 rainfall characteristics, wetting rates, vegetation cover and type, soil and crop management, and initial 146 and boundary conditions within the soil flow domain. Based on the definition of Hillel (1980) and Brutsaert 147 (2005) infiltration is defined as "the entry of water into the soil surface and its subsequent movement 148 through the soil profile". The sources of liquid water for infiltration include direct precipitation (rainfall, 149 dewfall, and snow melt), leaf drip and stem flow, irrigation, or runoff that was routed over the land surface 150 and re-infiltrates (a process termed runon). A detailed understanding of the primary controls on 151 infiltration rates and the onset of ponding with subsequent runoff, and their translation into model 152 equations, is of great importance at all scales. The accurate process representation of infiltration is also 153 essential for crop water use studies, the design of irrigation systems, and the optimal management of 154 water resources. Different approaches have thus been developed over the past decades to provide 155 quantitative tools able to describe and predict infiltration into porous media in soils, ranging from 156 empirical expressions, to analytical and numerical solutions of the basic flow equations.

Infiltration dynamics are determined by soil properties (hydraulic conductivity, sorptivity), the hydraulic gradients that drive flow, and initial and boundary conditions (Philip, 1957). Depending on the initial soil water content in the soil profile, the water supply rate and the corresponding soil wetting dynamics, all the available water can infiltrate in different amounts into the soil. Hence, these factors will influence the infiltration curve (the change with time of the infiltration rate during a wetting event) (Mein and Larson, 1973).

163 The infiltration capacity or potential infiltration rate of a soil, $q_{cap}(t)$, is the maximum rate at which the soil 164 surface can take up water for given initial conditions (Horton, 1940). The actual infiltration capacity is also 165 affected by the initial soil water content of the soil, but for practical considerations it may be considered 166 a time-dependent soil property where water inputs in excess of this maximum infiltration rate will pond 167 and likely generate runoff. For surface fluxes at rates lower than the soil's infiltration capacity, the realized 168 infiltration rate will depend upon the state of the soil (as shaped by the temporal history of the application 169 rates and the consecutive sequences of wetting and drying). Two infiltration regimes in unsaturated soils 170 can be distinguished and lead to different occurrence times of ponding and thus runoff generation: 171 constant water supply (occuring during irrigation or simulated rainfall) and variable rate supply (during 172 natural rainfall) as is shown in Figures 1 and 2, in terms of rates (top panel) or cumulative depths (bottom 173 panel; in this case capital symbols are used).

174 The dashed curves in Figure 1 and 2 represent the infiltration capacity, $q_{cop}(t)$ [LT⁻¹] or $Q_{cop}(t)$ [L], of a given 175 soil profile, the dotted line depicts the water supply rate, r(t) [L T⁻¹] or R(t) [L], for the constant 176 precipitation rate (Fig. 1) or for the variable precipitation rate one, as it is often the case during natural 177 rainfall (Fig. 2), and the solid line shows the actual infiltration rate, q(t) [L T⁻¹] or Q(t) [L], during these 178 events. In case of the constant r(t), all the applied water can infiltrate in the first stage of wetting (Fig. 1), 179 and q(t) = r(t). Compared to $q_{cap}(t)$ corresponding to an unlimited water application rate, q(t) can be higher 180 than $q_{cap}(t)$ because the hydraulic gradients resulting from the unsaturated condition generated by the 181 limited wetting rate, r(t), are larger than the ones that result from the saturated condition inherent to the 182 unlimited wetting rate. However, both curves tend towards a similar "quasi-steady" infiltration rate 183 corresponding to a gradient of unity, but approach it at different rates resulting from the difference in the 184 rate of decrease of the hydraulic gradients corresponding to each wetting condition. As wetting 185 progresses, q(t) begins to decrease, and at the time of ponding, t_p , where the infiltration rate, $q(t_p)$ is 186 smaller than the wetting rate, $r(t_p)$, ponding occurs at the soil surface.



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Figure 1: (A) Illustrative representation of the infiltration capacity rate, $q_{cap}(t)$ (dashed curve) and the actual infiltration rate, q(t) (solid line) of a soil profile exposed to a rainfall event with constant intensity r(t) (dotted line). The time t_c denotes the moment where $q_{cap}(t)=r(t)$, while the time t_p denotes the ponding time where q(t)=r(t). Shifting the representation of $q_{cap}(t)$ by $t_0=(t_p-t_c)$ (dashed-dotted line) allows to estimate t_p . (B) Illustration of t_p in terms of the cumulative infiltration, with $I(t_p)=R(t_p)$. (C) Cumulative infiltration capacity $I_{cap}(t)$ (dashed line) and cumulative rainfall R(t) (dotted line). The ponding time t_p can be estimated by means of $I_{cap}(t-t_0)$ (dashed-dotted line).



Figure 2: (A) Illustrative representation of the infiltration capacity rate, $q_{cap}(t)$ (dashed curve) and the actual infiltration rate, q(t) (solid line) of a soil profile exposed to a rainfall event with variable intensity r(t) (dotted line). For low r(t) values below $q_{cap}(t)$, q(t)=r(t), and the result is that t_c is close to t_p . (B) Cumulative infiltration capacity $I_{cap}(t)$ (dashed line), cumulative actual infiltration, I(t) (solid line), and cumulative rainfall R(t) (dotted line). In this case, t_p cannot be estimated by means of $I_{cap}(t_p-t_0)$. The figure was adapted from Assouline et al. (2007).

204 In terms of cumulative infiltrating volumes of water (or water depths, which are volumes per unit area). 205 (Fig. 1-lower) Q(t) is always smaller than $Q_{cop}(t)$ even when q(t) was higher than $q_{cop}(t)$, indicating that the 206 concept of infiltration capacity corresponds to cumulative infiltration rather than to infiltration rates. 207 Since the wetting rate is constant, the picture in terms of infiltration rates (Fig. 1, upper) and cumulative 208 depths (Fig. 1, lower) provide similar condition for t_p . Corresponding to the time where Q(t) departs from 209 R(t). It is interesting to note; that if it is assumed that ponding occurs when r(t) exceeds $q_{cap}(t)$, t_p is underestimated (Fig. 1, upper). The infiltration regime under variable r(t) and the prediction of t_p is much 210 211 more complicated as q(t) depends on the pattern of r(t) (Fig. 2, upper). The picture is much simpler when 212 expressed in terms of cumulative depths (Fig. 2, lower). Assouline et al. (2007) have proposed a simple 213 method to estimate t_p under variable r(t).

214 The cases described in Figs. 1 and 2 represent one mechanism of runoff formation termed infiltration 215 excess or Hortonian overland flow (Horton, 1933). Another important mechanism corresponds to the 216 formation of a saturated topsoil layer that enhances runoff formation. This mechanism is termed 217 saturation excess or Dunne overland flow (Dunne, 1978, Freeze, 1980). Dunne overland flow occurs when 218 the soil reaches saturation from above, via direct precipitation, or below and no additional water supplied 219 from the top can be stored in the soil profile. This can happen, for example, when the local water table is 220 high or a hydraulically impeding layer close to the soil surface exists (causing a so-called 'perched' water 221 table). In general, the Dunne mechanism occurs in areas close to the channels of the drainage network of 222 a catchment or in areas in the low lying parts of a catchment where the depth to the water table is shallow. 223 It is therefore more common in humid climates. These saturated runoff source areas vary in size, 224 seasonally and during individual storm events. Therefore, they are often referred to as variable source 225 areas (VSA) (Dunne and Black, 1970), and the runoff generated on them as VSA runoff (as e.g. in the 226 TOPMODEL (Beven and Kirkby, 1979), which is implemented (sometimes in modified form) in many land 227 surface models. On the other hand, Hortonian overland flow is more common in semi-arid climates 228 (Entekhabi and Eagleson, 1989).

Infiltration theory, and related numerical and analytical solutions, was originally the domain of soil
physicists. Several reviews on different aspects of infiltration into soils have been published (Assouline,
2013, Barry et al., 2007, Clothier, 2001, Gardner, 1960, Hopmans et al., 2007, Parlange, 1980, Parlange et
al., 1999, Philip, 1969, Philip and Knight, 1974, Raats, 2001, Raats et al., 2002, Skaggs, 1982) and also
constitute key chapters in textbooks (e.g., Bear, 1972, Brutsaert, 2005, Childs, 1969, Chow et al., 1988,

Delleur, 2006, Hillel, 1998, Warrick, 2003). The fundamental concepts of infiltration have been applied in
hydrology to deal with the prediction of infiltration at the field scale (Corradini et al., 2011, Govindaraju
et al., 2012, Morbidelli et al., 2006), on hillslopes (e.g., Morbidelli et al., 2018), for heterogeneous soil
systems (Govindaraju et al., 2001), and to handle the impact of complex precipitation events and patterns
on infiltration (Corradini et al., 1994, Corradini et al., 1997).

239 With the advent of efforts to model the global water and energy cycles at the large-scale, infiltration 240 theory was taken up by the climate and hydrological modelling community. Largely due to the (originally) 241 limited computing power and the difficulty in defining spatially distributed and appropriately upscaled soil 242 parameters, simplifications and approximations of the infiltration process were introduced into the land 243 surface models (LSMs) embedded in weather and climate models. The main role of a LSM is to compute 244 the energy partitioning at the interface between land surface and atmosphere. At the land surface, net 245 radiation is converted into latent heat, sensible heat and ground heat flux, where the latent heat flux is 246 the equivalent of the evapotranspiration flux in the water balance, but in this case expressed in energy 247 units. The energy partitioning at the land surface directly affects the state of the atmosphere. For example, 248 the relative magnitude of the latent and sensible heat flux will modify atmospheric state variables such as 249 relative humidity and the height of the atmospheric boundary layer, which in turn will affect cloud forming 250 processes, and ultimately rainfall. Infiltration acts on this energy partitioning indirectly via its control on 251 soil moisture content. Near-surface soil moisture content is an important state variable in both the water 252 and energy balance. For example, it affects net radiation due to its effects on land surface radiative 253 properties, albedo and emissivity. Also, both soil evaporation and transpiration depend strongly on soil 254 moisture content. A reduction in soil moisture content will lower evaporation via a reduced soil-255 atmosphere vapour gradient, and decreased replenishment of water to the evaporation front due to 256 reduced hydraulic conductivity, whereas transpiration is affected via a decrease in root water uptake 257 during drought conditions. Finally, because soil thermal conductivity and heat capacity are functions of 258 soil moisture, infiltration also indirectly affects the soil heat regime. Anwar et al. (2018) showed that the 259 choice of the infiltration scheme had a significant effect on the simulated regional climate. The infiltration 260 scheme with the lower soil infiltration rate yielded a lower topsoil soil moisture that led to a lower latent 261 heat flux and a higher sensible heat flux resulting in a net warming effect within the simulation domain.

262 With regard to the simulation of infiltration a range of approaches at different levels of complexity 263 currently exists in these models.

Paniconi and Putti (2015) reviewed the last five decades of physically based numerical models in hydrology and addressed the treatment of infiltration from local via hillslope to catchment scale. They focused on the flow path heterogeneity, whereby the analysis has been focused on the non-linearity and upscaling in hydrology with a specific focus on numerical methods used in hydrological models and related computational challenges. They briefly discussed the seminal work of Horton (1933), Betson and Marius (1969), and Dunne and Black (1970) in identifying the main mechanisms of runoff generation, which is closely related to the infiltration process.

271 Zhao and Li (2015) reviewed the different approaches to model land surface processes over complex 272 terrain. The main focus was on the role of grid scale spatial heterogeneity of land surface variables and 273 parameters (e.g., soil moisture content, net primary productivity, leaf area index (LAI), fraction of 274 vegetation cover) and the topographic impact on key atmospheric controls (e.g., precipitation, air 275 temperature, wind speed, air pressure). The role of infiltration and its different parameterization was 276 briefly addressed in relation to the spatial variability of soil hydraulic properties in complex terrains.

277 Clark et al. (2015) analyzed the state-of-the-art of infiltration processes in land surface models. They 278 concluded that the main challenges are in the appropriate treatment of the small-scale heterogeneity to 279 describe the large-scale fluxes of infiltration and surface runoff, and the need for an improved description 280 of wetting front dynamics, which may lead to improved simulations of infiltration and surface runoff 281 during heavy rainfall. More recently, Mueller et al. (2016) examined the potential of the land surface 282 models SWAP, JULES, and CH-TESSEL to produce surface runoff for intense rainfall events. Based on the 283 results, they recommend that future work should consider a correction of the maximum infiltration rate 284 in JULES and to investigate its numerical scheme in order to make it suitable for high vertical resolution. 285 Recently, Morbidelli et al. (2018) reviewed the role of slope on infiltration. They pointed out the need to 286 further develop upscaling approaches up to catchment and subgrid scale and to establish a theoretical 287 framework to describe infiltration on hillslopes to better explain experimental observations that have 288 become available in the recent years.

In this review, we will briefly recapitulate the main approaches and solutions derived from soil physical theory to describe infiltration processes at the point and field scale and the techniques used to numerically solve the infiltration processes, and finally to quantify the impact of spatial variability on infiltration. Hereby, we will focus on infiltration processes in non-frozen soils. We will present the infiltration approaches used in various land surface models and address how maximum infiltration capacity is quantified, how soil moisture and spatial variability of soil properties are parameterized, and how the areal saturation fraction, F_{sat} , important for Hortonian runoff, is estimated. We will also identify key soil parameters that affect the soil infiltration and runoff and present upscaling approaches for soil hydraulic parameters applicable to the grid scale of land surface models. Finally, we will present an outlook and future perspectives on modeling infiltration in land surface models.

299 **2. Quantitative Expression of the Infiltration Process at the Point Scale**

2.1. Basic Physical Models of Soil Water Flow and Infiltration

The chronological development of three main approaches in the conceptual modeling of infiltration inporous media is presented in the following.

303 Darcy (1856) formulated the first quantitative description of flow through a saturated porous medium,
 304 known as *Darcy's Law*:

$$305 \qquad J = -K_s \frac{\partial H}{\partial z}$$
[1]

where *J* is the Darcian flux of water $[L T^{-1}]$ at time *t* [T], *K*_s is a proportionality constant characterizing the medium and named "the saturated hydraulic conductivity" $[L T^{-1}]$, and $\frac{\partial H}{\partial z}$ [-] is the hydraulic gradient calculated form the differences in total hydraulic head (*H*) and the (vertical) distance *z* [L] within the saturated porous medium (in saturated soils, the total head *H* is the sum of pressure (*h*) and elevation heads (*z*)).

Buckingham (1907) proposed to extend Darcy's law to unsaturated water flow, where the actual water content in the porous medium, θ , is lower than its maximum value at saturation, θ_s . The main assumption is that the constant saturated hydraulic conductivity value, K_s , could be replaced by a function of soil water content, θ , or matrix potential, h, as the characteristic of the unsaturated porous medium. That function was named "the unsaturated hydraulic conductivity function", and given the symbol $K(\theta)$ or K(h). Following the notation of Eq. (1), the resulting unsaturated flow equation resulting from Buckingham's assumptions is:

318
$$J = -K(h)\frac{\partial H}{\partial z} = -K(h)\left(\frac{\partial h}{\partial z} + 1\right)$$
 [2]

where z [L] is the vertical coordinate being positive upward and z = 0 representing a prescribed reference
level. In this case, the total head H is the sum of the matrix potential in head units, h, and the gravitational
head z.

Finally, Richards (1931) combined the flow equation of Buckingham (1907) (Eq. 2) and the principle of continuity assuming an infinitely mobile air phase in the soil (zero resistance to air flow). The resulting well-known and widely used one-dimensional expression for the vertical water flow is given by:

325
$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right]$$
[3]

Eq. 3 requires the definition of an additional characteristic of the porous medium, this is the soil water retention curve (WRC), where the actual water content is a function of the matrix potential, $\theta(h)$.

The $\theta(h)$ and K(h) functions represent the hydraulic properties of the porous medium. An up-to-date presentation of the mathematical expressions (e.g., Brooks and Corey, 1964, Van Genuchten, 1980) used to quantify these properties in soils can be found in the review of Assouline and Or (2013).

331 The Brooks and Corey (1964) retention function is given by:

332
$$S_e(h) = \left(\frac{h}{h_c}\right)^{-\lambda_p}; h < h_c$$
 [4]

333 $S_e(h) = 1$; $h \ge h_c$

334 where h_c is the matric potential at air entry value [L⁻¹], λ_p is a dimensionless pore size distribution index 335 [-], *h* is the pressure head [L], and S_e is the effective saturation [-] given by:

$$S_e = \frac{\theta - \theta_r}{\phi - \theta_r}$$
[5]

337 where S_e is the effective saturation [-], θ is the actual water content [L³ L⁻³], θ_r is the residual water content 338 [L³ L⁻³], and ϕ is the porosity [L³ L⁻³], which can be related to θ_s as the saturated water content.

339 The corresponding unsaturated hydraulic conductivity function is expressed by:

340
$$K = K_s S_e^{(3+2/\lambda_p)}$$
 [6]

341 where K_s is the saturated hydraulic conductivity [L T⁻¹].

342 The water retention function proposed by Van Genuchten (1980) is given by:

343
$$\theta(h) = \theta_r - \frac{\theta_s - \theta_r}{\left(1 + |h/h_c|^{n_{vg}}\right)^m}$$
[7]

where *m* is a shape factor [-] often assumed to be related to n_{vg} by $m = 1 - 1/n_{vg}$. This function is continuous in *h* and present an inflection point, making it more appropriate for application in numerical solutions.

Applying the model of Mualem (1976) to Eq. 7 leads to the following unsaturated hydraulic conductivityfunction:

349
$$K(h) = K_s S_e^l \left[1 - \left(1 - S_e^{1/m} \right)^m \right]^2$$
 [8]

350 where *l* is a fitting parameter depending on the soil type [-].

351 The Richards equation (Eq. [3]) represents the actual physical model that can be used to simulate and 352 illustrate the infiltration process in porous media. It addresses only the macroscale behavior and is valid 353 for a representative volume for which the prescribed hydraulic properties can be applied. The solution of 354 the Richards equation requires the definition of initial and boundary conditions. When water is ponding 355 at the soil surface, infiltration is governed by the hydraulic head at the soil surface, a concentration type 356 boundary condition known also as a Dirichlet boundary condition. When the water application rate is 357 below the soil infiltration capacity, a flux or Neumann boundary condition can be applied at the soil 358 surface. Since Eq. [3] is highly nonlinear due to the non-linear character of the hydraulic conductivity 359 function $[K(h) \text{ or } K(\theta)]$, analytical solutions can only be derived for specific initial and boundary conditions, 360 and with knowledge of the soil hydraulic properties. Consequently, solutions to practical soil water flow 361 problems generally require the use of numerical schemes designed to solve partial differential equations.

362 **2.2. Empirical Infiltration Equations**

The necessity to describe quantitatively such a crucial hydrological process as infiltration combined with the complexity of the solution of the flow equation (Eq. [3]) led to the development of empirical expressions relating infiltration rate, q, to time t. From Fig. 1 it can be seen that, for a constant water supply, r(t), infiltration rate q(t) gradually decreases and tends towards a steady final infiltration rate, q_{f} . Consequently, the different forms of the suggested empirical equations describing infiltration are all 368 monotonically decreasing functions based on exponential or power law decays, for which the parameters369 do not generally have a physical meaning and are evaluated by fitting to experimental data.

In general, there are two main families of equations used to describe the infiltration process, whereby one is based on the original formulation of Horton (1941) and the other on those presented by Kostiakov (1932). Over time, both equations were modified and extended by various authors such as the Kostiakov model by Lewis (1937), Mezencev (1948), Smith (1972), Parhi et al. (2007), and Furman et al. (2006) to account for different initial and boundary conditions. The original formulation proposed by Horton (1941) predicts an exponential decay of the infiltration flux *q* over time *t* by:

376
$$q(t) = q_f + (q_i - q_f)e^{-\alpha_K t}$$
 [9]

where *q* is the infiltration rate [L T⁻¹], q_f is the final (constant) infiltration rate [L T⁻¹], q_i is the initial infiltration rate [L T⁻¹], and α_K is the decay constant (T⁻¹). For $t \to \infty$, q_f can be related to the hydraulic conductivity of the wetted soil layer.

380 On the other hand, Kostiakov (1932) introduced a power law equation with two fitting parameters n_K 381 and β_K in the form of:

382
$$q(t) = q_f + n_K \beta_K t^{(\beta_K - 1)}$$
 [10]

383 where n_K and β_K depend on initial and boundary conditions of the soil system.

2.3. Analytical and Semi-analytical Infiltration Description

385 Compared to the empirical models, analytical and semi-analytical equations based on Richards equation 386 were also developed, wereby Philip (1957) and Philip (1969) presented the first analytical solution to the 387 Richards equation. It considers infiltration as a sorption process with a perturbation generated by the 388 presence of gravity. Therefore, this method corresponds by definition to the first stages of infiltration into 389 a relatively dry soil profile where gravity plays only a minor role. It can therefore be expected to be 390 applicable for small and intermediate values of time (Brutsaert, 2005, Hillel, 1998). Because the original 391 solution, in the form of a power series, diverges for large values of time, Philip (1957) proposed to use a 392 truncated version of the original solution, considering the first two terms of the series:

393
$$q(t) = \frac{1}{2}S_{op}t^{-\frac{1}{2}} + A$$
 [11]

394 where S_{op} is defined as the soil sorptivity [L T⁻²], t is time [T], and A is a fitting parameter [-]. Note that Eq. [11] is equivalent to Eq. [10] for $\beta_K = 1/2$, $n_K = S_{op}$, and $q_f = A$. For long infiltration times (during ponded 395 infiltration), the term A approaches the value of K_s. Philip (1969) and Talsma and Parlange (1972) have 396 397 shown that even for long infiltration times (of practical interest), the inequality: $\frac{1}{3}K_s \leq A \leq \frac{3}{3}K_s$ holds. The 398 spatial vertical water content distribution in the soil profile following infiltration and wetting is quite 399 complex and can be illustrated by Fig. 3. Experimental results from Davidson J et al. (1963) and Rubin and 400 Steinhardt (1964) have shown the sigmoid-like nature of the distribution of $\theta(z)$ (here, the data of 401 Davidson J et al. (1963) are depicted in Fig. 4).



402

Figure 3: Illustration of the 2-D spatial distribution of soil moisture content within a wetted soil profile
during infiltration (left panel) and its corresponding soil moisture profile (right panel). AA' refers to a
vertical transect depicted on the right hand side of the left panel. Or et al. Classnotes with permission.

Green and Ampt (1911) presented an approach that is based on fundamental physics but make strong assumptions about the soil hydraulic properties and the shape of $\theta(z)$. Their key assumption is the presence of a sharp infiltration front moving downward with time, instead of the sigmoid distribution of water content with depth representing a more realistic wetting front as shown in Fig. 3 and 4. The presented infiltration function integrated macroscale physical entities such as pressure head differences over depth, soil porosity, and saturated hydraulic conductivity over the wetter soil layer. The Green-Ampt model, for the case of ponding infiltration with a negligible ponded water depth at the surface, is 413 represented by an implicit expression for the infiltration rate, q(t), which needs to be solved iteratively 414 for the cumulative infiltration Q(t):

415
$$q(t) = K_s \left(\frac{h_f(\theta_s - \theta_i)}{Q(t)} + 1 \right)$$
[12]

416 where Q(t) is the cumulative infiltration [L] at time t [T], h_f is the capillary head at the wetting front [L], K_s

is the soil saturated hydraulic conductivity [L T⁻¹], and θ_t is the initial water content of the soil profile. The

418 matrix head h_f is related to soil hydraulic properties (Bouwer, 1964, Neuman, 1976).



419

422

420 **Figure 4:** Infiltration into Hesperia sandy loam soil (inially air-dry) showing the soil water content θ with 421 depth, and the propagation of the wetting front with time during infiltration (reprinted with permission

from (Davidson J et al., 1963).

Generalized and exact solutions for *Q*(*t*) were developed by Parlange et al. (1985), Parlange et al. (1982), Haverkamp et al. (1990), Swartzendruber (1987), Ross et al. (1996), Barry et al. (1995), and Barry et al. (2005). Selker and Assouline (2017) present a simple explicit solution for the position of the wetting front in time based on approximating the term describing early infiltration behavior by means of the sum of gravitational flow and the exact solution for capillary imbibition.

428
$$q(t) = K_s \frac{A_f K_s + \sqrt{\frac{n_f K_s h_f}{2t}}}{1 + A_f \frac{K_s t}{n_f h_f} + \sqrt{\frac{2}{n_f h_f} K_s t}}$$
[13]

429 with A_f being a fitting parameter that can be approximated by (²/₃). For infiltration into a completely dry 430 soil profile $n_f = \theta_s - \theta_r$, whereas for a profile with known initial water content θ_i , $n_f = \theta_s - \theta_i$.

The result of Eq. [13] is within 1% of the exact implicit solution of vertical Green and Ampt infiltration Eq. [12]. Hence, the proposed approximation adds essentially no error to the Green and Ampt approach, but greatly simplifies computation of infiltration by allowing an explicit expression that is in theory easy to implement in LSMs.

For near-constant rainfall rates, q(Q) is independent of the applied rate r (Skaggs, 1982, Smith et al., 2002), and infiltration capacity at any given time depends only on the cumulative infiltration volume, regardless of the previous rainfall history. The time invariance of q(Q) holds true also when a layered profile or a sealed soil surface is considered (Mualem and Assouline, 1996, Smith 1990). This is an important characteristic of the infiltration process and the basis of the so-called Time Compression Analysis (TCA) for predicting the timing of ponding and runoff (Assouline et al., 2007, Brutsaert, 2005).

441 **2.4.** Numerical Solutions of Profile Scale Infiltration Processes

While the empirical, analytical, and semi-analytical models discussed above provide descriptions of the infiltration process for relatively simple conditions (e.g., a homogeneous soil profile, constant initial saturation with depth, constant ponding at the soil surface), the quantitative analysis of real-world infiltration problems (e.g., a layered soil profile, variable initial saturation, time-variable rainfall, limited ponding) can be obtained only using numerical solutions of the water flow equation (i.e., Richards equation (Eq. [3])). The reason lies in the fact that the highly nonlinear eliptic parabolic Richards equation cannot be solved analytically, apart from for a very limited number of cases.

Since the 1960s soil water balance models have been developed that quantify and predict infiltration insoil by numerically solving the Richards equation for different boundary conditions and resulted in a wide

451 range of software tools such as HYDRUS (Šimůnek et al., 2008), COUP (Jansson, 2012), DAISY (Hansen et al., 2012), and SWAP (van Dam et al., 2008), amongst many others. By using such models based on the 452 453 Richards equation along with sufficient vertical and temporal discretization, the infiltration rate and 454 occurrence of ponding should be a direct outcome of the numerical solution in the spatio-temporal 455 domain and do not have to be calculated 'externally' using any of the introduced empirical or (semi-) 456 analytical models above. Various simulations have been performed using HYDRUS-1D to demonstrate the 457 water infiltration into a 1D soil profile under natural boundary conditions (Šimunek and van Genuchten, 458 2008, Šimůnek et al., 2008, Šimůnek et al., 2016). The HYDRUS-1D model was selected for this purpose 459 since it is one of the most widely used and verified codes for unsaturated flow and solute transport 460 modeling (Scanlon, 2004) and the full set of simulations can be found at https://www.pc-461 progress.com/Downloads/Public_Lib_H1D/Using_HYDRUS-1D_to_Simulate_Infiltration.pdf.

462 Depending on the intensity of precipitation, both discretization in space and time need to be adapted to 463 the rainfall flux, whereby most current models rely on a predefined vertical discretization and only the 464 time discretization will be changed by an adaptive time stepping routine. In general, the typical size of the 465 vertical discretization is often smaller than one centimeter close to the soil surface in order to adequately 466 solve the Richards equation for rainfall events with high intensities. In some models the upper boundary 467 condition can be automatically switched from a flux boundary condition to a fixed pressure head 468 (Dirichlet) boundary condition during evaporation conditions to avoid the development of extreme 469 pressure head gradients close to the soil surface. This approach stabilizes the numerical solution of the 470 Richards equation. Additionally, the appropriate choice of temporal resolution of precipitation data is 471 extremely important to capture the generation of excess water (Hortonian excess). Finally, using daily 472 accumulated rainfall fluxes will lead to an under estimation of the generated excess water compared to 473 the use of highly resolved rainfall data (Mertens et al., 2002).

474 **2.4.1. Numerical Methods**

475 Most early applications of numerical methods for solving variably-saturated flow problems usually used 476 the classical finite differences method (e.g., Bresler, 1973, Bresler and Hanks, 1969, Hanks et al., 1969, 477 Rubin and Steinhardt, 1964). Integrated finite difference, finite volumes, and especially finite element 478 methods became increasingly popular in the seventies and thereafter (e.g., Huyakorn et al., 1986, 479 Neuman, 1973, Paniconi and Putti, 1994, Šimůnek et al., 2008), accompanying the fast development of 480 computers with increasing computational speed and memory. While finite difference methods are still used today in the majority of one-dimensional models, finite volume methods and/or finite element methods coupled with mass lumping of the mass balance term are usually used in two- and threedimensional models (e.g., Healy, 2008, Pruess, 1991, Šimůnek et al., 2008). An overview of these developments with respect to infiltration prediction is given in the review of Assouline (2013).

Furthermore, a number of LSMs use *semi implicit* numerical solutions to Richards one-dimensional partial differential equation (PDE) such as in Best et al. (2011), OLAM-SOIL (Walko and Avissar, 2008a), ORCHIDEE (de Rosnay et al., 2002), and ISBA-SURFEX (Boone et al., 2000, Decharme et al., 2011). Conventional methods for solving this highly non-linear equation inevitably lead to numerical and accuracy challenges that impact their hydrological performance.

490 **2.4.2. Governing Flow Equations**

In general, the Richards equation can be formulated, and thus solved numerically, in three different ways: water content (θ) based (often also denoted as the diffusivity form), pressure head (h) based, and in terms of a mixed formulation, when both θ and h appear simultaneously in the governing equation as shown in Eq. [3]. The most popularly used vadose zone flow models currently utilize the mixed formulation of the Richards equation and solve this equation using the mass-conservative method proposed by Celia et al. (1990).

497 **2.4.3. Boundary Conditions**

Infiltration rates for a point source infiltration process can be obtained by numerically solving the Richards
equation for an appropriate upper (soil surface) boundary condition (BC). In general, two types of BCs can
be used to simulate the infiltration process, i.e., the Dirichlet or Neumann BC. The Dirichlet (pressure head
based) BC fixes the pressure head, *h*, at the soil surface (*z* = 0) to a value *h*₀ [L], which can be either constant
or variable with time:

503
$$h(z,t) = h_o(t)$$
 at $z = 0$ [14]

The value for h_0 can either be negative (e.g., for tension disk infiltration), zero, or positive (ponded infiltration). The majority of empirical, analytical, and semi-analytical models discussed above represent conditions with zero (or slightly positive) pressure head at the soil surface. The Neumann (flux based) BC fixes the water flux (infiltration), q, at the soil surface to a required water flux, q_0 [LT⁻¹], which can again be either constant or variable with time:

509
$$-K\left(\frac{\partial h}{\partial z}+1\right) = q_0(t)$$
 [15]

510 where q_0 is negative for infiltration and positive for evaporation when the *z*-axis is defined positive upward 511 if *z* is defined negative over depth. If water is allowed to build up on the soil surface after the onset of soil 512 surface ponding, a "surface reservoir" boundary condition may be applied (Mis, 1982, Šimůnek et al., 513 2008, van Dam et al., 2008):

514
$$-K\left(\frac{\partial h}{\partial z}+1\right) = q_0(t) - \frac{dh}{dt}$$
 [16]

The flux q_0 in Eq. [16] is the net infiltration rate, i.e., the difference between precipitation and evaporation. Based on Eq. (16) the height h(0,t) of the surface water layer (ponding height) increases due to precipitation and reduces because of infiltration and evaporation of the ponding layer.

518 Kollet and Maxwell (2006) closed the problem of variably saturated groundwater flow, infiltration, and 519 surface water flow by applying flux and pressure continuity conditions at the top boundary leading to a 520 free surface overland flow boundary condition

521
$$-K\left(\frac{\partial h}{\partial z}+1\right) = \frac{\partial \|h,0\|}{\partial t} - \nabla \mathbf{v} \|h,0\| + q_0(t)$$
[17]

where v is the depth averaged velocity vector [LT⁻¹], that can be expressed in terms of Manning's equation (e.g., in Chow et al., 1988) to establish a flow depth-discharge relationship.

524

525 The Dirichlet (Eq. 14) and Neuman (Eq. 15) boundary conditions are system-independent boundary 526 conditions for which prescribed quantities (i.e., pressure heads or water fluxes) do not depend on the 527 conditions of the soil profile, its saturation status, or its infiltration capacity. These boundary conditions 528 thus may not properly describe real-world conditions, in which infiltration or actual soil evaporation rates 529 depend on the conditions of the soil profile and its saturation status, which may limit infiltration or 530 evaporation. In many applications, neither the flux across nor the pressure head at a boundary is known 531 a priori but follows from interactions between the vadose zone and its surroundings (e.g., the 532 atmosphere). External meteorological conditions thus control only the potential water flux across the soil 533 surface, while the actual flux also depends on the prevailing (transient) soil moisture conditions near the 534 surface. This occurs, for example, when the precipitation rate exceeds the infiltration capacity of the soil, 535 resulting in accumulation of excess water on top of the soil surface and surface runoff, depending upon soil properties and on topographic conditions (for 2 and 3-D representation). Subsequently, the infiltration rate 536 537 is no longer controlled by the precipitation rate, but instead by the soil infiltration capacity.

538 Such conditions may be best described using system-dependent boundary conditions, which take soil 539 moisture conditions and the hydraulic conductivity of the soil near the soil surface into consideration. For 540 example, in HYDRUS-1D, such a system-dependent BC is called an "atmospheric" BC. For these conditions, 541 the soil surface boundary condition may change from a prescribed flux to a prescribed head type condition 542 (and vice-versa). The numerical solution of Eq. 3 is then obtained by limiting the absolute value of the 543 surface flux by the following two conditions (Neuman et al., 1974):

544
$$\left|-K\frac{\partial h}{\partial z}-K\right| \le i_p$$
 [18]

545 and

$$546 h_A \le h \le h_s [19]$$

where i_p is the maximum potential rate of infiltration or evaporation under the current atmospheric conditions [LT⁻¹], and h_A and h_s are, respectively, minimum (i.e., for evaporation) and maximum (i.e., for infiltration) pressure heads at the soil surface allowed under the prevailing soil conditions [L]. When one of the endpoints of Eq. 19 is reached, a prescribed head boundary condition will be used to calculate the actual surface infiltration or evaporation flux.

552 The value for h_A is determined from the equilibrium conditions between soil water and atmospheric water 553 vapor (e.g., Feddes et al., 1974). The value of h_s is usually set equal to zero, which represents conditions 554 when any excess water on the soil surface is immediately removed via runoff once ponding is reached. In 555 this case, the Neumann BC (Eq. 15) is switched internally in the model to the Dirichlet BC (Eq. 14) with h=0556 once ponding is reached and then back to the Neumann BC once rainfall stops (during redistribution) and 557 the pressure head decreases below zero. When h_s is allowed to be positive, it then represents a layer of 558 water, which can form on top of the soil surface during heavy rains before initiation of runoff. In such 559 case, the Neumann BC (Eq. 15) needs to be switched to the Dirichlet BC (Eq. 14) similarly as above, but 560 the surface pressure head value h is calculated using the surface reservoir BC. Once rainfall stops, 561 infiltration (calculated for a Dirichlet BC) continues until all water from the accumulated water layer has 562 infiltrated when the BC is switched back to the Neumann BC.

563 2.4.4. Vertical and Temporal Discretization

The numerical solution of the highly nonlinear Richards equation requires relatively fine spatial (on the 564 565 order of cm) (Vogel and Ippisch, 2008) and temporal (on the order of minutes) discretization. Optimal 566 spatial and temporal discretization depends strongly on the intensity of precipitation/evaporation/infiltration and the nonlinearity of soil hydraulic properties, as well as on 567

568 numerical stability criteria, involving hydraulic or thermal diffusivity (see e.g., Best et al., 2005).
569 Simulations with high flux rates and strong nonlinearity of soil hydraulic properties require finer
570 discretization in both space and time. Most current vadose zone, including land surface, models rely on a
571 predefined vertical discretization, which is constant in time, while only the time discretization changes
572 during simulations by an adaptive time stepping routine.

573 Spatial discretization should be made relatively small at locations where large hydraulic gradients are 574 expected. Such a region is usually located close to the soil surface where highly variable meteorological 575 factors can cause rapid changes in soil water contents and corresponding pressure heads. Hence, it is 576 generally recommended to use relatively thin soil layers (small discretization) near the soil surface and then 577 to gradually increase their thickness with depth to reflect much slower changes in pressure heads at deeper 578 depths.

3. Upscaling Approaches Towards Larger Scales

Infiltration considered at larger scales is heavily affected by the heterogeneity of the soils and the land surface. Assouline and Mualem (2002, 2006) explicitly demonstrate the impact of heterogeneity, introduced by a combined effect of impervious areas and spatial variability in soil properties, on infiltration. Figure 5 shows the results in terms of the infiltration rate (q(t)) curves for a homogeneous and a heterogeneous field exposed to a constant rainfall rate.



585

586

Figure 5: Mean infiltration in a heterogeneous (solid line) vs. a homogeneous (dashed line) field.

587 Accounting for field spatial variability leads to shorter ponding times and to a more gradual decrease of 588 the infiltration flux with time (Smith and Hebbert, 1979). Consequently, surface runoff will appear earlier 589 in heterogeneous fields than in homogeneous ones. This results from the fact that part of the 590 heterogeneous field has much lower hydraulic conductivity than that of the homogeneous one and this 591 generates the early runoff. As LSMs typically incorporate infiltration at grid sizes from meters to hundreds 592 of kilometers, scaling approaches are necessary to account for sub-grid heterogeneity at the model 593 resolution. Also, parameters relevant for infiltration, as well as experiments for direct infiltration 594 measurements, are typically observed and performed at the point-scale (see Section 2). Therefore, scaling 595 approaches are needed to translate the measurements to adequately address infiltration characteristics 596 at larger scales. Two general strategies are discussed in the following, (i) the scaling of infiltration-related 597 properties and (ii) the scaling of infiltration fluxes themselves. We have chosen this categorization rather 598 than a scale based categorization as several of the methods proposed below, such as e.g. similarity scaling, 599 aggregation, and Bayesian upscaling, can be applied at a range of scales. Figure 6 shows the different 600 upscaling approaches to obtain effective parameters at the scale of LSMs. We distinguish four different 601 categories: i) the LSM upscaling approaches that either assign uniform soil properties to a dominant soil

602 class or use pdfs of parameters that reflect subgrid variability, ii) parameter upscaling methods, iii) 603 similarity upscaling methods, and iv) stochastic upscaling methods. The last three approaches have been 604 mainly developed for upscaling from the field to catchment scale, while the first one involves downscaling 605 the parameters from grid to point scale, before upscaling the resulting infiltration from point to grid scale. 606 Within the LSM upscaling approaches, three main methods can be distinguished: (1) Uniform upscaling 607 assuming the soil hydraulic parameters are constant (2) Empirical upscaling that use pdfs to define F_{sat} and I_{max} that are then further used to calculate grid-cale infiltration, and (3) Physical upscaling in which 608 609 infiltration is calculated at point-scale and pdfs are used used to upscale it at grid-scale.

3.1. Upscaling Spatially Heterogenous Parameters Relevant for Infiltration

LSMs need input parameters at the grid scale, i.e. estimates of effective parameters to quantify 611 612 hydrological and energy balance fluxes, and to generate soil infiltration-related properties such as water 613 storage at the grid cell level (see Section 2). In order to adequately represent nonlinear relationships 614 between model parameters and states and fluxes, it is generally agreed upon that spatial scaling ideally 615 should take place after the model has been run. However, this is also a matter of computational resources, 616 which are limited and generally do not afford simulations at the support, which is the area or volume over 617 which a measurement is made or a state variable defined. LSMs driven for global or continental 618 applications typically require upscaling of information that is available at higher resolution to scales of a few to tens of kilometers. Here, a simplification of the landscape heterogeneity by dominant class 619 620 selection (e.g., USDA soil classes) or simple parameter averaging typically does not account for nonlinear 621 relationships of sub-grid processes and may introduce important biases on specific LSM variables, 622 including infiltration and runoff (Boone and Wetzel, 1999).



623

Figure 6: Schematic overview of different upscaling methods of soil parameters (Original LSM upscaling
approach, Parameter upscaling, Similarity scaling, and Stochastic upscaling) described in section 4., 3.1,
3.21, and 3.2.2.). Differences in the infiltration model used are indicated by different colors.

Another method proposed by Noilhan and Lacarrère (1995) consists to compute grid-scale land surface parameters according to observed soil textures (sand and clay) aggregated from the high resolution and using continuous relationship derived from textural classification of Clapp and Hornberger (1978) or Cosby et al. (1984). The scaled effective parameters are often dependent on the spatiotemporal patterns of the unsaturated system at the smaller scale and are not simply a function of the average parameter values obtained from measurements.

- 633 General focus was placed on upscaling soil hydraulic parameters, because significant spatial variability of
- these properties has been reported earlier by Nielsen et al. (1973), Warrick and Nielsen (1980), Peck
- 635 (1983), and Logsdon and Jaynes (1996). In most of these cases, the field saturated hydraulic conductivity,

*K*_s, was log-normally distributed (Reynolds and Eldrick, 1985, Russo et al., 1997, White and Sully, 1992).
However, steady-state infiltration fluxes and soil surface water content are distributed either normally or
log-normally (Cosh et al., 2004, Kutilek et al., 1993, Loague and Gander, 1990, Sisson and Wierenga, 1981,
Vieira et al., 1981). Several studies have dealt with modeling the effect of spatial variability of soil hydraulic
properties on infiltration (Assouline and Mualem, 2002, Dagan and Bresler, 1983, Govindaraju et al., 2006,
Milly and Eagleson, 1988, Sivapalan and Wood, 1986, Smith and Hebbert, 1979, Warrick and Nielsen,
1980, Woolhiser et al., 1996).

643 While heterogeneity in soil hydrology properties, parameters, and boundary conditions is ubiqoutous, 644 understanding of sensitivity to different aggregation/upscaling methods is limited. Zhu and Mohanty 645 (2002a, 2002b, 2003, 2004, 2006), Zhu et al. (2006, 2004), and Mohanty and Zhu (2007) investigated in a 646 series of studies the suitability of various soil hydraulic parameter upscaling schemes by matching their 647 prediction performances with ensemble vadose zone fluxes (infiltration and evaporation) under different 648 hydroclimatic scenarios for horizontally and vertically heterogeneous soil systems. Their synthetic 649 experimental results showed that soil texture, geological layering, groundwater depth, surface/profile soil 650 moisture status, vertical flux direction (infiltration versus evaporation), hydraulic parameter statistics 651 (correlations and spatial structures), root distribution in the soil profile, and topographic 652 features/arrangements conjointly determine the "upscaled" pixel-scale soil hydraulic parameters for the 653 equivalent homogeneous medium that delivers the same amount of flux (infiltration or evaporation) as 654 the natural heterogeneous medium. Thus, different homogenization algorithms (rules) for different 655 hydrologic scenarios and land attribute complexities were suggested for parameter upscaling. Several 656 approaches have been proposed in the literature to upscale soil hydraulic properties from the point to 657 larger scales in order to obtain effective properties (Vereecken et al., 2007a), which are discussed in the 658 following.

659 3.1.1. Topography-based Aggregation

Expanding the power average operator of Yager (2001), Jana and Mohanty (2012a, 2012b, c) coarsened the soil hydraulic parameters to the model grid scale in the attempt to study remote sensing based soil moisture distribution at the watershed scale (Little Washita). Two types of aggregating methods were combined in this topography-based aggregation technique. By combining the features of both mode-like and mean-type aggregating methods, the power average technique provided an ideal tool in scaling of soil hydraulic parameters for soil pedons. Power averaging operator across a number of spatial nodes use a support function based on linear distances in different Cartesian coordinates allowing data clustered around a particular value to combine nonlinearly while being aggregated. Generally, soil pedons clustered
 around a location tend to have similar properties, that correlation decreases as the distance between two
 points increases. In other words, the aggregating method considers the mutual support the pedons extend
 to each other when clustered.

671 **3.1.2. Homogenization**

672 Homogenization by spatially averaging the soil hydraulic parameters is a simple way of upscaling. Numerical studies such as those presented by Zhu and Mohanty (2002b) and Mohanty and Zhu (2007), 673 674 and observational studies such as those of Jana and Mohanty (2012b) examined the impact of areal heterogeneity of soil hydraulic parameters at the model grid scale on the ensemble response of hydrologic 675 676 fluxes. In particular, arithmetic, geometric, and harmonic averages of the soil hydraulic parameters were 677 tested with different parameter correlation structures. Findings of these studies suggested that different 678 averaging schemes should be used for different soil hydraulic conductivity parameters and functional 679 forms.

680 3.1.3. Similarity Scaling

Another method for scaling is based on the theoretical framework of geometric similarity for porous media introduced by Miller and Miller (1956). The basic idea is, that porous media, which are geometrically similar in their microscopic arrangement of particles, differ only in terms of their characteristic length scale λ_{sc} . The underlying assumption is that the hydraulic behavior of a porous medium can be transformed to the behavior of a reference medium by scaling (Nielsen et al., 1998). This scaling factor α_{sc} is defined as the ratio between the characteristic length λ_{sc} of a geometrically similar soil and the characteristic length of the reference soil λ_r :

$$688 \qquad \alpha_{SC} = \frac{\lambda_{SC}}{\lambda_r}$$
[20]

This approach can also be used for spatial scaling of soil hydraulic properties (Mohanty, 1999, Shouse and Mohanty, 1998). Zhu and Mohanty (2006) used Miller-Miller scaling in combination with a onedimensional infiltration equation based on the Haverkamp et al. (1990) model to derive effective hydraulic parameters at the grid scale of LSM and global climate models (GCMs). Heterogeneity of soil hydraulic parameters was considered in the horizontal dimension and the infiltration process was described using the concept of parallel stream tubes without lateral interaction. They found that the variability in Miller-Miller scaling factors had a strong influence on the effective grid cell infiltration than the saturated water 696 content and the ponding depth, which reflects micro-topography. This approach was also implemented 697 by Montzka et al. (2017) to generate an optimized soil hydraulic properties data base at coarse global grid 698 resolution of 0.25° from the soil texture information system SoilGrids1km of Hengl et al. (2014). Further 699 information about similarity and Miller-Miller scaling in terms of scaling infiltration processes is given in 690 Section 3.2.1.

701 3.1.4. Bayesian Upscaling

Considered as a calibration method at the remote sensing footprint scale, the Markov Chain Monte Carlo (MCMC) based upscaling algorithm introduced by Das et al. (2008) provides an alternative to derive the upscaled effective soil hydraulic parameters from a time-series of soil moisture observations and stochastic information of the fine scale soil hydraulic parameter variability. The Bayesian framework produces probability distributions of the effective (pixel-scale) soil hydraulic parameters, where preexisting knowledge about the local scale soil parameters (e.g., from Soil Survey Geographic (SSURGO) database) can be combined with dynamic hydrologic observations and model outputs.

709 Kim and Mohanty (2017) proposed a more general approach by accounting for the effects of mixed 710 (weighted) physical controls (covariates) as well as the interactions between the controls on soil moisture 711 distribution and subsurface flow including lateral flow between grid cells. They used a Bayesian averaging 712 scheme for effectively estimating the contributing ratios (weights) for the physical controls and their 713 interactions. This scheme provide proper weights that show how the controls contribute to describing the 714 spatial variability of soil moisture and thus effective soil hydraulic properties. This approach underpins the 715 concept of hydrologic connectivity, based on probability of connected local pathways of surface and 716 subsurface flow, by which emergent catchment-scale behavior is depicted. The physical control based 717 connectivity index approach can be easily adopted in land surface hydrologic and biogeochemical models 718 leading to an Earth System Modelling (ESM) framework, where geophysical attributes such as geology, 719 ecotones, and topography are (will be) the primary drivers for water, carbon, and energy cycle.

720 **3.1.5 Machine Learning Based Upscaling**

Pedotransfer functions have been used as inexpensive alternatives for estimating soil infiltration and hydraulic properties using soil textural and bulk density information at the local scale. Expanding the concept of pedotransfer function to estimate landscape-scale soil hydraulic properties, Sharma et al. (2006) developed Artificial Neural Networks (ANN)-based pedo-topo-vegetation transfer functions with good success by adding topographic and vegetation characteristics to soil textural and bulk density 726 information. Advancing the idea within a Bayesian framework, Jana et al. (2008) and Jana and Mohanty 727 (2011) developed multi-scale Bayesian Neural Network (BNN) based pedotransfter functions. Using BNN, they upscaled/downscaled soil hydraulic parameters using soil texture and structure data at one scale, to 728 729 simulate the key soil moisture contents related to soil water retention at another. In that study, training 730 inputs to the BNN consisted of the percentage of sand, silt, and clay, and the bulk density of the soil, and 731 DEM and vegetation data, while the targets were the soil water content at 0 (saturation), 0.33 (field 732 capacity), and 15 (wilting point) bar. Using MCMC techniques, the BNN provides a distribution of the 733 output parameter instead of a single deterministic value. Recently, Montzka et al. (2017) used 734 pedotransfer functions to derive effective spatial distribution of scaling factors and mean properties of 735 soil hydraulic properties that can be used in LSMs to quantify the effect of spatial variability on infiltration 736 fluxes.

737 3.1.6 Multiscale Parameter Regionalization

738 The Multiscale Parameter Regionalization (MPR) method proposed by Samaniego et al. (2010) is a two-739 step approach with initial regionalization and subsequent upscaling. The regionalization establishes a 740 priori relationships between model parameters and distributed basin predictors at the fine scale, leading 741 to linear or nonlinear transfer functions. These functions are used as global parameters to reduce 742 overparameterization and ease transferability. Soil texture and land cover can be used as predictors for 743 infiltration (Samaniego et al., 2010). The upscaling towards coarser scales is performed by a selection or 744 combination of upscaling operators such as arithmetic mean, maximum difference, geometric mean, 745 harmonic mean, and majority. With this approach, the sub-grid variability is used for facilitating 746 transferability towards ungauged and uncalibrated regions for improved model parameterization. 747 Samaniego et al. (2017) analyzed the applicability of the MPR approach for several LSMs.

748 **3.1.7 Other Parameter Scaling Approaches**

Other parameter scaling methods are fractal approaches (e.g., Tyler and Wheatcraft, 1990) and the scaleway approach (e.g., Vogel and Roth, 1998). Although, they have been used over small watersheds, they have strong limitations (Meng et al., 2006). Stochastic upscaling or aggregation methods statistically allow to better account for landscape heterogeneity conditions. Stochastic upscaling makes use of geostatistical descriptors of spatial variables and quantify a probability distribution for each state variable at larger scales by stochastic perturbation rather than a deterministic quantity (see Section 3.2.2). Govindaraju et al. (2006) suggested a semi-analytical model to compute the space-averaged infiltration at the hillslope scale when spatial variability in both soil properties and rainfall intensity are accounted for. The soil spatial heterogeneity was characterized by a log-normal distribution of the saturated hydraulic conductivity, while the rainfall spatial heterogeneity was simulated by a uniform distribution between two extreme rainfall intensities (low and high). At each location, the soil saturated hydraulic conductivity, K_s , and the rainfall intensity was assumed to remain constant during the rainfall event. The main finding was that ponding time decreases with the increase in the coefficient of variation of K_s (see also Figure 5).

762 Other researchers also developed and evaluated methods that are potentially applicable for transfering 763 infiltration parameterizations across scales. Hailegeorgis et al. (2015) evaluated four regionalization 764 methods for continuous streamflow simulation. Their regional calibration method uses the maximum 765 weighted average of a performance measure such as Nash-Sutcliff Efficiency to identify specific parameter 766 sets per sub-pixel by the DREAM algorithm (Vrugt et al., 2009). Another method uses the regional median 767 of each parameter for regionalization, where a limitation is that the correlation structure between 768 parameters is lost. Scaling by the nearest neighbor approach includes the assumption that spatial 769 proximity in terms of Euclidian distance explains parameter similarity. The physical similarity approach 770 assumes that similarity of regions in physical attributes such as land use, cumulative distribution functions 771 of terrain slopes, and/or soil types can explain their response in the hydrological variable.

The potential of most of these upscaling methods has not yet been tested in currently used land surface models. As highly resolved soil information becomes available that allows to parametrize subgrid variability, several of the above presented methods may prove to be valuable in estimating effective soil properties controlling infiltration processes at the pixel scale of land surface models. First results using e.g. the multi-scale parameterization method and similarity approach show great potential in parameterizing key hydraulic properties at the grid scale of LSM.

778 **3.2. Upscaling Infiltration Processes**

In order to upscale infiltration processes themselves rather than providing a method for the averaging of infiltration-related parameters as discussed above, besides scaling the Richards equation for infiltration (Sadeghi et al., 2012, Warrick and Hussen, 1993), the Miller-Miller similarity can be applied. The stochastic upscaling of infiltration is based on the frequency distribution of infiltration-related parameters and allows for a computation of effective infiltration fluxes using semi-analytical approximations.

784 3.2.1 Similarity Scaling

Besides providing a method for the averaging of infiltration-related parameters as presented in Section 3.1.3 similarity scaling can also be applied for a reduction of the number of parameters in the analytical or semi-analytical infiltration equations, which in turn also reduces the data requirement. Within the similarity scaling approach for infiltration, the infiltration data consists of a set of scaling factors, one for each location or grid cell, and an average infiltration function. In the following, mainly two examples of similarity scaling for infiltration are presented. The first example Sharma et al. (1980). is based on the similiraty scaling of cumulative infiltration *Q* [L], which is estimated over time *t* (Philip and de Vries, 1957):

792
$$Q(t) = S_{op}t^{1/2} + ACt.$$
 [21]

where $S_{op,i}$ and AC_i are the parameters fitted to each of the infiltration measurements, *i*, within a region. Sharma et al. (1980) use two alternative approaches to realize the scaling of cumulative infiltration: i) either by determination of two separate scaling factors for the sorptivity and steady state infiltration, or ii) by determination of a single optimized scaling factor. For the first approach, the two scaling factors α_{Sop} and α_{AC} [-], for sorptivity S_{op} [L T^{-0.5}] and steady state infiltration AC [L T⁻¹], respectively, were calculated according to

799
$$\alpha_{Sop,i} = \left(\frac{S_{op,i}}{\langle S_{op} \rangle}\right)^2$$
 [22]

800 and

801
$$\alpha_{AC,i} = \left(\frac{AC_i}{\langle AC \rangle}\right)^{1/2}$$
, [23]

802 where $\langle S_{op} \rangle$ and $\langle AC \rangle$ represent the respective mean values of those fitted infiltration parameters. The 803 scaling of the infiltration data was subsequently performed by:

$$804 \qquad Q^* = \alpha Q \tag{24}$$

805 and

806
$$t^* = \alpha^3 t$$
, [25]

807 where Q^* and t^* identify the scaled cumulative infiltration [L] and time [T], respectively, and scaling factor 808 α is either α_{Sop} or α_{AC} . At this point, both scaling factors α_{opt} and α_{AC} can be used to scale the cumulative infiltration data. However, both attempts, using either α_{opt} or α_{AC} , fail to arrange the scaled infiltration data near the reference cumulative infiltration curve $\langle Q \rangle$ defined by $\langle S_{op} \rangle$ and $\langle AC \rangle$. For the second scaling approach, a single scaling factor α_{opt} was derived by least-squares fitting (using Eqs. [24] and [25]). The sum of squares, SS, between scaled cumulative infiltration and reference cumulative infiltration, given by

814
$$SS = \sum_{t_i^*} \left(Q_{t_i^*}^* - \langle Q \rangle_{t_i} \right)^2$$
 [26]

was minimized by adjusting α_{opt} based on the cumulative infiltration measurements available at each timestep t_i for each of the multiple measurements. Finally, with this second scaling approach all the measurements reasonably coalesced about the reference cumulative infiltration curve.

818 By using Eq. [26], Sharma et al. (1980) depart from the geometric similarity proposed by Miller and Miller 819 (1956), which would require that $\alpha_{S_{op}}$ and α_{AC} are identical. A scaling methodology following the second 820 approach (Eq. 26) is empirical in nature and usually referred to as functional normalization (Tillotson and 821 Nielsen, 1984). Nonetheless, it is still relevant since it provides a mathematical framework for the handling 822 of Philips' infiltration in terms of spatial variability. Eqs. [24] to [26] can be used to account for the 823 variability in infiltration, when only the variance of the scaling factors and the mean infiltration curve are 824 known. Furthermore, this approach provides an opportunity to lump both infiltration parameters AC_i and $S_{op,i}$ into a single scaling parameter $\alpha_{SC,i}$ for each soil. Yet, to the best of our knowledge, such an 825 826 approach has not been implemented in any land surface or hydrological model. However, for the spatial 827 scales of LSMs, it remains unclear how appropriate scaling parameters could be derived and implemented 828 in practice.

The frequency distribution of α_{opt} determined by Sharma et al. (1980) had a mean of about 1, as expected, and a standard deviation of 0.58. The spatial distribution of α_{opt} did not show a distinct pattern, which was explained by Loague and Gander (1990) later on, as they determined a spatial autocorrelation length of less than 20 m for infiltration in the catchment under consideration. This in turn would support a purely stochastic approach to the variability of infiltration. However, this conclusion is based on the assumption of the occurrence of vertical fluxes only. Hopmans (1989) simplified the scaling of Philips' infiltration suggested by Sharma et al. (1980) by substituting Eqs. [22] and [23] into Eq. [21]. Accordingly, the scaled instantaneous infiltration q^* [L T⁻¹] yields:

838
$$q^*(t) = \alpha_{SC}^{1/2} \langle S_{op} \rangle t^{-1/2} + \alpha_{SC}^{-2} \langle AC \rangle$$
 [27]

where q^* is the scaled infiltration rate [L T⁻¹], and $\langle S_{op} \rangle$ [L T^{-0.5}] and $\langle AC \rangle$ [L T⁻¹] represent the parameters 839 840 of the reference infiltration curve, now determined by non-linear regression to all infiltration 841 measurements available. Hopmans (1989) also performed functional normalization according to Tillotson 842 and Nielsen (1984) with the modified empirical three-parameter infiltration equation of Kostiakov (see 843 Eq. [10]). Both scaling approaches were successful and the author stressed that the attractiveness of this 844 lies in the potential to lump the spatial variability of infiltration into a single parameter, which, for 845 example, allows for correlation with other environmental variables. Furthermore, it potentially removes 846 any inter-correlations between the infiltration parameters.

Haverkamp et al. (1998) provide inspectional analyses of Miller-Miller similarity scaling for infiltration according to the theories provided by Green and Ampt (1911), Philip (1957), and Talsma and Parlange (1972). However, the analyses presented by Haverkamp et al. (1998) remain at a theoretical level and were not tested in any practical application.

851 3.2.2 Stochastic Upscaling

852 A stochastic approach to upscale infiltration can be implemented via Monte-Carlo simulations for any type 853 of infiltration equation and any given distribution of relevant parameters. This has been demonstrated, 854 e.g., by Smith and Hebbert (1979) and Sharma and Seely (1979). A sufficient number of random samples 855 needs to be drawn from a given distribution of infiltration parameters and after computation of every 856 Monte-Carlo model realization the average and/or standard deviation of predicted infiltration can be 857 obtained. However, due to the assumption that the infiltration process is ergodic, large sample sizes are 858 usually required resulting in a rather large computational demand, which in reality prohibits any practical 859 application in large-scale studies involving hydrological models or LSMs. Notwithstanding, many semi-860 analytical solutions to infiltration problems are still validated against Monte Carlo results (e.g., Corradini 861 et al., 2002, Craig et al., 2010, Govindaraju et al., 2001).

862 Starting with the infiltration theory according to Philip (1957), while making some considerable 863 approximations, Sivapalan and Wood (1986) provided semi-analytical solutions to calculate average infiltration over a gridbox for two cases. For the first case, a spatially constant rainfall rate, and a lognormal distribution of saturated hydraulic conductivity K_s were assumed. In the second case, a spatially variable rainfall rate and spatially uniform distribution of K_s were considered. In both cases, run-on was not accounted for and the soil profiles were assumed to be vertically homogeneous. The approximations derived by Sivapalan and Wood (1986) were tested against Monte-Carlo simulations, but an in-depth analysis of the uncertainties was not presented. Moreover, due to the mathematical complexity of the approximations, practical application was not feasible.

871 Smith and Goodrich (2000) simulated the ensemble behavior of infiltration according to Parlange et al. (1982) by making use of Latin hypercube sampling. They assumed that the log-normal probability density 872 873 functions of K_s and capillary parameter G were divided into n equal sub-areas and infiltration was 874 computed using the average of each sub-area. The areal average infiltration was then given as the equally 875 weighted sum of all subdivisions. This method does not involve any analytical solution and has the 876 advantage of a significantly reduced computational demand as compared to the Monte Carlo technique. 877 Govindaraju et al. (2001) assume spatial autocorrelation of log-normally distributed saturated hydraulic 878 conductivity and provide semi-analytical solutions to the Green-Ampt equation based on series expansion. 879 As a follow-up, the semi-analytical solutions of Govindaraju et al. (2001) were combined by Corradini et 880 al. (2002) with a kinematic wave expression to account for run-on effects.

881 Craig et al. (2010) provide approximations for the estimation of average infiltration rate $\langle q \rangle$ [L T⁻¹] 882 according to the Green-Ampt approach as a function of precipitation rate J_w [L T⁻¹] and mean saturated hydraulic conductivity, $\langle K_s \rangle$, and standard deviation, σ_{Ks} , of a standard log-normal distribution, $f_k(K_s)$, of 883 884 saturated hydraulic conductivity, K_s . They estimated a dimensionless error term ε for J_w , K_s , and X, whereby 885 X represents a dimensionless time parameter computed from time t, J_w, and α_{wf} . This last variable α_{wf} 886 is defined as the product of the absolute value of wetting front suction head and the difference between 887 saturated water content and initial water content at the beginning of the infiltration event. Finally, the 888 averaged infiltration rate, $\langle q \rangle$, is approximated by:

$$889 \qquad \langle q \rangle = \frac{J_w}{2} \operatorname{erfc}\left(\frac{\ln(J_w X) - \langle K_s \rangle}{\sigma_{ks}\sqrt{2}}\right) + \frac{1}{2X} \exp\left(\langle K_s \rangle + \frac{\sigma_{ks}^2}{2}\right) \operatorname{erfc}\left(\frac{\sigma_{ks}}{\sqrt{2}} - \frac{\ln(J_w X) - \langle K_s \rangle}{\sigma_{ks}\sqrt{2}}\right) + J_w \int_0^{X(t)} \varepsilon(X(t), k_s) \cdot f_k(k_s) dk_s \qquad [28]$$

According to the authors a comparison between the semi-analytical upscaling approach given in Eq. [28] with Monte-Carlo simulations revealed errors of less than 3%, which appears to be acceptable for any practical purpose. The authors also provide approximations of infiltration for a given normal distribution
893 of aggregate parameter α_{wf} . From Monte-Carlo simulations Craig et al. (2010) concluded that the 894 heterogeneity in K_s is of much greater relevance than the heterogeneity in α_{wf} .

Craig et al. (2010) upscaled the Green and Ampt equation to a basin or (LSM) grid cell. Thereby, the upscaled Green Ampt equation is based on the information of the distributions of saturated hydraulic conductivity, K_s , and/or the initial soil water deficit of the basin or grid cell. Additionally, preferential flow, which is defined as the uneven and rapid movement of water through the soil, characterized by regions of enhanced flux e.g., wormholes, root holes, cracks, can be also incorporated by considering a bimodal distribution of K_s by:

901
$$\langle q \rangle = \int_0^\infty \int_0^\infty (X(t, \alpha_{GA}), K_s) f_{k\alpha_{GA}}(K_s, \alpha_{GA}) d\alpha_{GA} dK_s$$
 [29]

902 with

903
$$X = 1/\left(1 + 1\left(\frac{J_W}{\alpha_{GA}}\right)t\right)$$
[30]

904 with $\alpha_{GA} = |h_f|(\theta_s - \theta_i)$, where h_f is the pressure head at the wetting front [L], θ_s is the saturated water 905 content and θ_i is the water content at the wetting front [L³ L⁻³]. The ponding time can be calculated as:

906
$$t_p = \frac{\alpha_{wf}K_s}{J_w(J_w - K_s)}$$
 [31]

This approach also allows calculating of the saturated land surface fraction in a basin or LSM grid cell. To
 our knowledge, none of the proposed methods related to stochastic upscaling have been tested or used
 in full LSM/hydrological models.

Finally, Choi et al. (2007) developed a three-dimensional volume-averaged soil moisture transport model (VAST) based on Richards equation to account for local scale variation of topographic attributes such as elevation, slope, and curvature on subsurface soil moisture fluxes and thus also the infiltration flux. In this approach, the coordinate system $x_i \in \{x, y, z\}$ is replaced by $x_i^* \in \{x, y, z^*\}$ where z^* follows the terrain elevation defined as:

915
$$z^* = Z_g - z$$
 [32]

with Z_g as the ground surface elevation [L]. The local terrain surface slopes, $S_{x_l}^*$, are defined as:

917
$$S_{x_l}^* = \left(\frac{\partial Z_g}{\partial x}\frac{\partial Z_g}{\partial y} - 1\right)$$
[33]

918 Second-order Taylor expansion of the hydraulic conductivity and diffusivity with respect to soil moisture 919 were formulated and substituted in a diffusion, pressure based Richards equation and the soil water 920 content and terrain slope at any point were approximated by a first-order perturbation approach. Scale 921 dependent functions are used to characterize sub-grid variability incorporating statistical properties that 922 relate the dependence of soil moisture variability to terrain attributes. The covariance between soil water 923 content and terrain slopes is defined as:

924
$$\langle \theta' S'_{x_l} \rangle = \rho \sigma_{\theta} \sigma_{S_{x_l}}$$
 [34]

where p is the correlation coefficient between the terrain slope and the soil water content. The correlation
coefficient was expressed by Choi et al. (2007) as:

927
$$\rho = \gamma_1 + \gamma_2 \left(\frac{\langle \theta \rangle}{\theta_s}\right) + \gamma_3 \left(\frac{\langle \theta \rangle}{\theta_s}\right)^2$$
[35]

928 where γ_1 , γ_2 , and γ_3 are fitting parameters estimated from observations. Note, that other approaches are 929 available to estimate the variance of soil water content (e.g., Choi et al., 2007, Qu et al., 2015, Vereecken 930 et al., 2007a).

931 Choi et al. (2007) combined this modelling approach with a 1D diffusion wave model for surface overland 932 flow, called it the conjunctive surface-subsurface flow model (CSSF) and proposed it for use in mesoscale 933 climate simulations. CSSF was tested through implementation in the common land model (CLM) (Oleson et al., 2008) using a set of offline simulations for catchment scale basins around the Ohio Valley region. 934 935 They showed that CSSF simulated a strong contribution of the effects of surface or overland flow depths 936 of water on infiltration estimates that led to an increased baseflow generation. In addition, a better 937 representation of the surface subsurface flow processes improved the representation of soil moisture 938 spatial variability and may improve the partitioning of energy at the land surface.

939 4. Infiltration Processes in Land Surface Models

In the following, we provide an overview of how widely used land surface models (LSMs) represent
infiltration processes at the global scale. Therefore, we selected 12 LSMs, namely: (1) OLAM-SOIL (Walko
et al., 2000), (2) ParFlow-CLM (Kollet and Maxwell, 2006, 2008a), (3) ORCHIDEE rev4783 (d'Orgeval et al.,
2008, Ducharne et al., 2017), (4) Catchment land surface model (CLSM) (de Lannoy et al., 2014, Ducharne
et al., 2000, Koster et al., 2000), (5) ISBA-SURFEX (Boone et al., 2000, Decharme et al., 2011, Decharme et
al., 2016, Decharme and Douville, 2006), (6) Noah-MP version 3.0 (Niu et al., 2011a, Schaake et al., 1996),

(7) JULES version 4.6 (Best et al., 2011, Clark et al., 2011), (8) CLM4.5 (Oleson et al., 2013), (9) CABLE
(Decker, 2015, Kowalczyk et al., 2013, Kowalczyk et al., 2006a, Wang et al., 2011), (10) SSiB (Li et al., 2010,
Sun and Xue, 2001b, Xue et al., 1991, Xue et al., 1996, Zhan et al., 2003), (11) CH-TESSEL (Balsamo et al.,
2009, Entekhabi and Eagleson, 1989), and (12) JSBach version 3.0 (Hagemann and Stacke, 2015, Roeckner
et al., 2003). All models are listed in Table 1 and the labeling is used throughout the appendix for
consistency.

First, we review how these LSMs address the challenge of treating infiltration processes in a large grid cell, and associated runoff generation. Second, we review how infiltration processes are treated numerically in different LSMs, considering approaches ranging from empirical to analytical equations or direct solution of the Richards equation with appropriate numerical schemes, boundary conditions, and vertical discretization. These approaches have been introduced in the previous sections.

957 **4.1. Grid Scale Infiltration Processes**

958 In this section, we focus on parameterization of infiltration and runoff generation processes and their 959 definition at the grid scale. These include the maximum infiltration rate, the characterization of the soil 960 water content distribution at the grid cell level, the characterization of grid cell heterogeneity with respect 961 to infiltration controls, and the saturated surface fraction. Although, most LSMs use a Richards' type 962 formulation to describe the soil water flow at the grid scale, it is used primarily to redistribute soil water 963 vertically in the profile rather than for calculation of infiltration rates at each time step. This is justified by 964 the computationally demanding solution of the pressure head at the land surface required for obtaining 965 accurate and stable solutions of the Richards equation. This calculation is particularly demanding during 966 high intensity rainfall events, where accurate solutions require very small spatial and temporal 967 discretization (see Section 2.4.4) leading to very high computational demand. Various parametric 968 approaches have been devised in LSMs to handle the process of infiltration efficiently within the 969 constraints of data availability (e.g., spatially available K_s values), to avoid such computational burden. 970 However, the implementation of Richards based solution for infiltration allows for: 1) direct calculation of 971 excess water flux (e.g., rainfall) that cannot infiltrate, 2) a physically-based determination of the time to 972 ponding, and 3) direct accounting for the effect of variable soil properties on infiltration at the grid cell 973 (when such information is available). Table 1 gives an overview of twelve different LSMs and their 974 numerical treatment of infiltration processes. Four of the twelve LSMs derive infiltration rates directly 975 from solving the Richards equation in its mixed form (ISBA-SURFEX, OLAM-SOIL, CLSM, and ParFlow-CLM)

and thus do appear only in some of the following sections dealing with specific issues of grid-scale parameterization of infiltration and runoff generation. Here, it has to be noted that most reviewed LSMs (except OLAM-SOIL and Parflow-CLM) are designed to be used globally, with typical grid-cell size of 0.5° or more. These models first define uniform soil parameters at the grid-cell (Table 3), used to calculate either infiltration, or Hortonian and Dunne runoff, at the point-scale. In the latter case, grid-scale infiltration is defined as the as the incoming water that does not run off.

982 4.1.1. The Maximum Infiltration Rate in LSM

983 In LSMs, the maximum infiltration rate is used to partition the water flux reaching the land surface into 984 infiltrable flux and excess water that generates surface runoff. In the subsequent, we will focus on 985 infiltration of vegetated or bare land surfaces and exclude glaciers, lakes, and urban areas. An interesting 986 example is provided by Entekhabi and Eagleson (1989), who used a Darcy based approach to estimate the 987 maximum infiltration rate or infiltrability for a heterogenous grid cell in a land surface model. They defined 988 surface runoff, q_s , as the sum of Hortonian infiltration excess ($P_x - f^*$ for $P_x > f^*$ and s < 1, i.e., the 989 first term on the right hand side in Eq. [36]) and Dunne saturation excess (the second term on the right 990 hand side of Eq. [36]) where saturation excess is equal to P_{χ} when $s \ge 1$:

991
$$q_s = \frac{1}{\kappa} \left[\int_0^1 \int_{f^*}^\infty (P_x - f^*) f_{P_x}(P_x) dP_x f_s(s) ds + \int_1^\infty \int_0^\infty (P_x) f_{P_x}(P_x) dP_x f_s(s) ds \right]$$
[36]

where, P_{χ} (ML²T⁻¹) is the flux of water incident at the soil surface, f^* the infiltrability of the first soil layer, 992 993 s is effective relative saturation, κ is a scaling factor needed to redistribute the global climate model 994 (GCM) grid scale precipitation over the scale of precipitation events, and f represents the spatial 995 probability density function (pdf) of the respective variables (rainfall and relative saturation). The first 996 term on the right hand refers to the amount of point precipitation intensity that exceeds the infiltration 997 rate of the soil, f^* , and therefore, represents the maximum infiltration rate at that moment in time. The 998 second term on the right hand side refers to the rainfall that falls on saturated surfaces and cannot 999 infiltrate.

1000 Based on Buckingham-Darcy equation they derived f^* as:

1001
$$f^* = K_s v s + K_s (1 - v)$$
 [37]

1002 where $v = \frac{dh}{ds}\Big|_{s=1} \frac{1}{\Delta z}$ and *h* is the matric potential [L], Δz the thickness of the first soil layer [L], *s* refers to 1003 to the effective relative saturation ((θ/θ_s) , and K_s is the saturated hydraulic conductivity (L T⁻¹). For 1004 gravitational flow v = 0 and hence $f^* \approx K_s$. It is important to state that K_s is assumed to be uniform for 1005 a grid cell.

1006 Other, more empirically based approaches have been implemented in LSMs to quantify the maximum 1007 infiltration rate to determine the excess water for surface runoff. LSMs differ in the way they define this 1008 maximum infiltration rate and the input parameter needed to estimate the infiltration flux. An overview 1009 of the different equations used in LSMs to estimate I_{max} is given in Table 2. Appendix A2 provides a more 1010 detailed presentation of the concepts and equations. In general, all LSMs that use I_{max} require, in some 1011 way or another, information about the actual soil water status of the land surface. In Noah-MP and CLM 1012 this is embedded in the saturated water fraction, Fsat (see Section 4.1.4). H-TESSEL and CH-TESSEL require 1013 knowledge about the actual and maximum water content of the first 50 cm of the soil profile to calculate 1014 Hortonian infiltration. ORCHIDEE, JULES and ISBA-SURFEX require information on the soil hydraulic 1015 conductivity to estimate I_{max}. CLSM does not use the concept of a maximum infiltration rate but assumes 1016 that the amount of water that can infiltrate over a certain time at the catchment scale is a function of the 1017 model's dynamically varying spatial moisture fields.

1018 Based on the detailed description provided in Appendix A2 on how maximum infiltration rate is estimated 1019 in LSMs, and the information provided in Table 1 on the numerical simulation of soil water flow at grid 1020 cell scale, we conclude that currently used LSMs parameterize infiltration processes by 1) estimating the 1021 saturated area in a grid cell to calculate Dunne saturation excess. All precipitation that falls on the 1022 saturated surface fraction of a grid cell becomes immediately available for runoff and does not infiltrate 1023 into the soil profile. 2) calculating the unsaturated land surface area available for Hortonian infiltration 1024 excess, and 3) using different approaches to simulate the maximum amount of water that can enter the 1025 soil during a certain time step, any excess being Hortonian infiltration excess.

No	LSM	Key References	Model time stepping	Vertical resolutionof the first compartment	Temporal resolution of precipitation input	Form of Richards equation used for 1D water movement	Infiltration rate from solution of Richards equation	Is ponding allowed based on pressure head?	Impact of lower boundary (LB) on infiltration	Approaches to point-scale infiltration	Approaches to grid-scale infiltration
1	OLAM-SOIL	1	less than a day (approx. 1 min to 6 hr)	2 to 5 cm	minutes	diffusivity form	Yes	Yes	LB of soil model is impermeable but >100 meters deep. Water table governed by Richards Eqn.	Richards Eqn. is coupled with surface water (ponding) upper boundary condition. Infiltration occurs when infiltration capacity will be exceeded	Uniform upscaling of infiltration
2	ParFlow-CLM	2, 3	variable	10 layers for first 3 m, additional 5 layer for next 100 m ⁵	variable	mixed form	Yes	Yes	Richards equation is solved globally (saturated and variably saturated conditions); different types of BCs can be used (Dirichlet, Neumann, gravity drainage)	runoff occurs if precipitation exceeds K_s	Uniform upscaling of infiltration
3	ORCHIDEE rev4783	4, 5	less than a day (30 min)	1 mm top layer, 11 layers in total	30 minutes	diffusivity form	No	No	By controling the soil moisture profile and therefore infiltration capacity	runoff occurs if precipitation exceeds $$K_{\rm s}$$	exponential pdf on ${\it K}_{\rm s}$
4	Catchment land surface model (CLSM)	6, 7, 8	less than a day (typically set to <1 hr)	1 cm for Richards equation in off- line simulations, 2 to 5 cm for catchment scale simulations.	hourly	mixed form	Yes ^b	No	Water table depth influences the soil moisture profile and therefore infiltration rates	runoff occurs if water table depth aboce surface or precipitation exceeds infiltration capacity	Richards Eqn. combined with TOPMODEL formulations to derive parameters for catchment-scale vertical moisture transfer
5	ISBA-SURFEX	9, 10, 11, 12	less than a day (down to 5 min)	0.01 m (by default but user can modify this)	maximum 3 hours but can be smaller depending on available data	mixed form	Yes*	No	the default is free drainage (hydraulic conductivity in lowest model layer) except when ISBA is coupled to a ground water model, in which capillary rise can occur into the soil from GW.	runoff occurs if precipitation exceeds Ks (Horton) or soil is saturated (Dunne)	 F_{sot} based on reflected power pdf on soil moisture capacity (Dümenil and Todini, 1992) or TOPMODEL approach
6	Noah-MP version 3.0	13, 14	Less than a day	four layers: 0.1 m, 0.3 m, 0.6 m und 1.0 m	offline mode 30 min to 1 hour. In coupled mode down to seconds	diffusivity form	No	No	no impact due to free drainage LB	runoff occurs if precipitation exceeds Ks (Horton) or soil is saturated (Dunne)	exponential pdf on precipitation, and Topmodel approach for F_{sat}
7	JULES version 4.6	15, 16	less than a day (typically 1hour but set by user)	flexible, set by user. Standard top layer = 10 cm.	flexible but never longer than 1 day. Usually between 1 to 6 hours	diffusivity form	No	No	When topmodel approach is used, there is an additional deep water store below the soil column, in which saturated conductivity is assumed to reduce exponentially with depth.	runoff occurs if precipitation exceeds Imax=βKs (Horton) or soil is saturated (Dunne)	TOPMODEL approach for F _{sor}
8	CLM4.5	17	less than a day (30 min)	increasing layer thickness with depth, upper layer = 1.75 cm	3 to 6 hours	(form is not provided)	No	Yes	no impact of LB	runoff occurs if precipitation exceeds Ks (Horton) or soil is saturated (Dunne)	TOPMODEL approach for F _{sot}
9	CABLE	18, 19, 20, 21	Fixed, depending on forcing data or coupling model time step.	Increasing layer thickness with depth; first layer 2.2 cm; soil thickness 4.6 m.	depending on forcing data or coupling model time step.	diffusivity form	No	No	Infiltration depends on vertically averaged relative saturation over the grid cell, which includes the lowest soil layer.	air space in first three soil layers is filled from the top with infiltration water at the beginning of timestep.	gamma pdf on soil moisture
10	SSiB	22, 23, 24, 25, 26	less than a day	increasing layer thickness with depth, upper layer = 1.75 cm	30 min or hourly	diffusivity formn	No	No	by interaction of baseflow and the overlying soil layers	runoff occurs if precipitation exceeds K_s	exponential pdf on precipitation
11	CH-TESSEL	27, 28	one hour or less	increasing layer thickness with depth, upper layer = 7 cm	flexible but never longer than 6 h offline. Typically 3-hourly or hourly offline and shorter/equal to atmospheric timestep when coupled	diffusivity form	No	No	no impact of LB	runoff occurs if soil moisture exceeds capacity	F _{set} based on reflected power pdf on soil moisture capacity (Dümenil and Todini, 1992)
12	JSBACH version 3.0	29, 30	less than a day (hourly)	6.5 cm	hourly, daily	diffusivity form	No	No	no impact of LB	runoff occurs if soil moisture exceeds capacity	F _{sor} based on reflected power pdf on soil moisture capacity (Dümenil and Todini, 1992)

* Calculation of infitration rate from solution of Richards equation is done only for small time steps. For large time steps and intense rain events, a Green Ampt based approach can permit infitrated water to attain several layers during a time step.
* Drameters for catchment-scale vertical motisture transfer between surface and root zone, and root zone and catchment deficit, are derived from detailed Richards equation simulations conducted off-line combined with TOPMODEL formulations.
* Parameters for retrainal discretizations in general flexible and can be set by the user, given example is used as standard setting in Terrs/sMP

¹ Walko et al. (2000), ² Kollet and Maxwell (2006), ⁴ Kollet and Maxwell (2006), ¹ d'Orgeval et al. (2010), ⁵ Ducharme (2017), ⁶ Koster et al. (2000), ⁷ Ducharme et al. (2014), ⁶ Boena et al. (2006), ¹⁰ Decharme and Douville (2006), ¹⁰ Decharme et al. (2011), ¹¹ Checharme et al. (2015), ¹⁰ Kowalcryk et al. (2011), ¹¹ Checharme et al. (201

1026

1027 **Table 1:** Overview of LSMs and their numerical treatment of infiltration process.

1028 With respect to Hortonian infiltration excess, the majority of the LSMs use an empirical parameterization 1029 of Imax. The vertical redistribution of the amount of infiltrated water in most LSMs is based on a diffusion 1030 form of the Richards equation. A primary consideration in using the simplified infiltration 1031 parameterization presented above is the large computational burden of solving the more accurate 1032 pressure head based Richards equation. Such a direct approach, however, has the advantage of obviating 1033 the need for defining maximum infiltration capacity, and that the amount of Hortonian infiltration excess 1034 and Dunne saturation excess are immediate outcomes of solving the Richards equation (albeit subgrid 1035 information and runoff-runon processes must be represented). CLSM overcomes the computational 1036 burden of the mixed form of the Richards equation by running detailed Richards equation simulations 1037 solely off-line prior to LSM runs in order to derive parameters of catchment-scale vertical moisture 1038 transfer using an amended TOPMODEL approach. Also, Walko et al. (2000) developed a global LSM (part 1039 of OLAM-SOIL) capable of calculating infiltration processes using a pressure head based Richards 1040 equations and highly resolved spatial information of soil properties.

4.1.2. Spatial Heterogeneity in Soil Water Content Using Probability Densities

Characterization of subgrid soil moisture variability in LSMs is especially important to estimate the 1042 1043 generation of Dunne saturation excess. In this section, we will focus on the different approaches used in 1044 land surface models to quantify heterogeneity in soil water content in respect of quantifying infiltration-1045 runoff processes at the grid scale level. These approaches are based on the underlying assumption that 1046 spatial variability in soil water content and derived properties such as soil water storage or soil water 1047 deficit can be described by probability density functions (pdf) without considering their spatial patterns 1048 nor specific locations. Different types of pdfs have been proposed and used in land surface models such 1049 as standard reflected power distribution functions, Gamma functions, and exponential functions.

Several researchers used standard reflection power distributions functions to describe spatial variability
 of soil water content and soil water content dependent variables that affect infiltration. These functions
 are a special case of the more general beta distribution function written as:

1053
$$f(x; \alpha_G, \beta_G) = \frac{\Gamma(\alpha_g + \beta_G)}{\Gamma(\alpha_G)\Gamma(\beta_G)} x^{\alpha_G - 1} (1 - x)^{\beta_G - 1} \qquad 0 \le x \le 1; \ \alpha_G, \beta_G > 0$$
[38]

1054 where $\Gamma(...)$ Is the Gamma function and α_G , β_G the parameters of the Gamma function. Moore (1985) 1055 was among the first to propose the probability-distributed model (PDM) as a concept to characterize 1056 spatial variability of soil water content related variables at the catchment scale. He used a standard reflected power cumulative distribution function to characterize the spatial variation of the storagecapacity, *c*, written as:

1059
$$F(c) = 1 - \left(1 - \frac{c}{c_{max}}\right)^b$$
 $0 \le c \le c_{max}; b > 0$ [39]

1060 with the corresponding density function

1061
$$f(c) = \frac{dF(c)}{dc} = \frac{b}{c_{max}} \left(1 - \frac{c}{c_{max}}\right)^{b-1}$$
 [40]

where *c* is the water storage capacity at a certain location defined as the depth of water that can be stored [L], c_{max} is the maximum water storage capacity [L], and *b* controls the spatial variability of storage capacity over the basin, whereby *b* = 0 indicates a constant value of the storage capacity and *b* = 1 means a capacity that follows a uniform distribution between 0 and c_{max} . Moore (1985) did not specify how to calculate the storage capacity from basic soil properties. Based on Eq. [40] we can derive the maximum water depth S_{max} (L) over the basin as:

1068
$$S_{max} = \int_0^{c_{max}} (1 - F(c)) dc = \frac{c_{max}}{b+1}$$
 [41]

1069 The concept proposed by Moore (1985) has been used in many land surface models using a bucket type 1070 of soil water model to characterize spatial variability of infiltration and storage capacity such as in VIC 1071 (Liang et al., 1994) or HD (Hagemann and Gates, 2003), or Richards equation based LSM (e.g., JULES, H-1072 TESSEL/CH-TESSEL). Clark and Gedney (2008) compared the PDM approach of Moore (1985) and a 1073 modified TOPMODEL approach in generating surface runoff using the MOSES (now JULES) LSM, by 1074 comparing model output against the observed stream flows in three catchments. TOPMODEL performed 1075 best as it allowed a better response to subsurface flow contributing to peak flows but also capturing 1076 slower changes in recession times. PDM only improved the calculation of the surface runoff without 1077 improving subsurface flow. In Appendix A1 we briefly describe the PDM scheme of Moore (1985).

1078 Rather than using a reflected power density function, Entekhabi and Eagleson (1989) proposed a two1079 parameter gamma pdf to characterize spatial heterogeneity of soil water content at the level of the grid
1080 cell:

1081
$$f_s(s;\alpha_c,\lambda_s) = \frac{\lambda_s^{\alpha_c}}{\Gamma(\alpha_c)} s^{\alpha_{c-1}} e^{-\lambda s}, \ \alpha_c,\lambda_s,s > 0$$
[42]

1082 where *s* is the mean surface layer point soil water saturation defined by

1083
$$s = \frac{\theta}{\theta_s}$$
 [43]

1084 with θ as the actual and θ_s defined as the saturated volumetric soil water contents [L³ L⁻³], respectively. 1085 The two parameter Gamma distribution, Γ , in Eq. [42] is related to *s* via:

1086
$$\lambda = \frac{\alpha_c}{\langle s \rangle}$$
 [44]

1087 where $\langle f(s) \rangle$ is the grid mean relative saturation of the surface soil layer [L³ L⁻³]. This concept has been 1088 implemented for example in the CABLE model (Decker, 2015).

For the CLSM, the basic land element is the (irregularly shaped) hydrological catchment rather than the GCM grid cell. A number of these catchments lie within a given cell, and grid-cell fluxes are computed through areal weighting of the component catchment fluxes. Within an individual catchment element, CLSM simulates a dynamic water table depth of which the distribution is related to catchment topography characteristics using the TOPMODEL formulation (Beven and Kirkby, 1979):

1094
$$d = \bar{d} - \frac{1}{\nu_K} \left(ln \frac{\alpha_T}{\tan \beta_T} - \bar{x} \right)$$
[45]

1095 where d is water table depth [L] (negative for ponding layers caused by rising groundwater), $ln(\alpha_T/tan\beta_T)$ is the 'topographic index' at the point in question, d is the mean water table depth [L], \bar{x} is the mean 1096 1097 catchment value of $ln(\alpha_T/tan\beta_T)$, α_T is the upstream area that contributes flow through a unit contour positioned at the point, and v_K is a parameter describing the decrease of saturated hydraulic conductivity 1098 1099 with depth. Each catchment is characterized by its topographic index distribution, which in effect is used 1100 to diagnose the spatial variability of soil moisture within the catchment. The information on soil moisture 1101 variability is used to define three distinct hydrological regimes: i) the wilting area, ii) the sub-saturated-1102 but-transpiring area, and iii) the saturated fraction. The definition of these three regimes is key to CSLM 1103 as different evaporation and runoff physics are applied to each.

4.1.3. Representing Spatial Heterogeneity of Surface Properties that Control

1105 Infiltration in a Single Parameter

Several land surface models use a single parameter in combination with pdfs in order to characterize the spatial heterogeneity of infiltration processes. Many of these pdfs, presented above, can be derived from Eq. [38], which was used in Section 4.1.2. to describe the spatial variability of soil water content and related variables. The estimation of this exponent (denoted as *B* or *b*) in such pdfs remains an open question as it cannot be immediately derived from available soil properties. Please note that this exponent has received sometimes a different notation in some LSMs. Liang and Xie (2001) used the "b" notation to describe the variability of soil and grid cell properties affecting Dunne excess saturation in the VIC model and the "B" parameter to describe the variability of soil and grid cell properties affecting Hortonian infiltration excess in the VIC model. Three main approaches have been reported in the literature to determine this exponent, from here on referred to as the *b* parameter, for simplicity.

1116 In the first approach, the *b* parameter is obtained by model calibration to available hydrological time 1117 series. Huang et al. (2003) present a brief discussion of the literature dealing with the estimation of the *b* 1118 parameter in the VIC model. They showed that the calibration approach suffers from the problem of 1119 equifinality, as so many other LSM calibration exercises. Furthermore, they did not manage to establish 1120 meaningful relationships between model parameters and physical characteristics of the catchment or 1121 regions.

In the second approach, the *b* parameter is derived from available soil and/or topographic information.
For example, Dümenil and Todini (1992) suggested to calculate the *b* parameter from the subgrid standard
deviation of topography by

1125
$$b = max \left[\frac{\sigma_h - \sigma_{min}}{\sigma_h - \sigma_{max}}; 0.01 \right]$$
 [46]

1126 where σ_h refers to the standard deviation of the topography within a model grid cell. Balsamo et al. (2009) 1127 stated that σ_h varies between 0.01 and 0.5 and σ_{min} and σ_{max} can be set to values proposed by van den 1128 Hurk and Viterbo (2003). On the other hand, Habets et al. (1999), in this case for the ISBA model, assumed 1129 the *b* parameter to be constant.

1130 The third option fits a pdf to the observed cumulative distributions of soil properties as a function of the 1131 occupied space in a grid cell or basin. Sivapalan and Woods (1995) fitted the so-called *Xinanjiang* 1132 distribution to data of soil profile depth to estimate the *b* parameter in the following equation:

1133
$$F_S(z^*) = 1 - (1 - Z/Zm)^b$$
 [47]

where F_s is the cumulative distribution function of the scaled infiltration capacity (scaled by its maximum value); *Z* is the soil profile depth to the bedrock [L] and *Zm* its maximum value of the bedrock depth within the gridcell [L]. Here, it is assumed that the available porosity is constant in space and time. To prove their concept, Sivapalan and Woods (1995) used a regionalized cumulative soil depth distribution for six 1138 landforms observed in the Serpentine catchment and obtained the best fit with a value of b = 4.03 and 1139 Zm = 10 m.

Huang et al. (2003) used a method based on a self-organizing neural network map combined with a *K*means clustering method to develop transfer functions that are able to transfer *b*-values of data rich to data poor areas. The data rich area was used to fit the relation to values of soil water capacity data derived from soil map information to the surface areas of catchments by:

1144
$$w = w_{max} [1 - (1 - A)^{1/b}]$$
 [48]

1145 where w and w_{max} are the point and maximum point soil water capacity, A is the area for which the soil 1146 water capacity is less than or equal to w, and b is defined as a soil water capacity shape parameter. In 1147 their study, Huang et al. (2003) used the STATSGO (Digital General Soil Map of the United States) database 1148 to represent the data rich areas. Here, it has to be noted that appropriate soil information at resolutions 1149 finer than 1 km is presently available, whereby the global SoilGrids1km 250m database of Hengl et al. 1150 (2014) is only one example. These new developments will allow estimating the value of the *b* parameter 1151 at high resolution globally, without the need of applying transfer approaches as proposed by Huang et al. 1152 (2003). Additionally, such highly resolved global map information combined with pedotransfer functions 1153 would allow to directly relate the b parameter to soil properties to be determined, as well as the subgrid 1154 variability depending on the size of the grid cells used in LSMs. This will be explained later on in Section 1155 4.1.5.3.

1156 **4.1.4. Estimating the Areal Saturation Fraction** *F*_{sat}

1157 Estimation of the areal saturation fraction, F_{sat} , as used for example in the equations listed in Appendix 1158 A2 Eqs. [A24 A35, A36, A40, A58, A50, A52, A56], is key in determining the contribution of Dunne 1159 saturation excess runoff and Hortonian infiltration excess runoff to the overall runoff generation of a grid 1160 cell in many LSM. In this section, we will discuss briefly the different approaches used in various LSMs. A 1161 correct representation of F_{sat} typically requires a good knowledge about subsurface properties like the 1162 depth to bedrock, the location of the groundwater table, soil porosity, and the actual state of the soil 1163 water content in the profile. One approach that is frequently used in LSMs is based on the assumption 1164 that the saturated fraction of a grid cell can be determined from topographical characteristics and the soil 1165 moisture status of a grid cell. This approach is closely related to the concept introduced in the TOPMODEL 1166 and adopted in many studies of infiltration runoff generation. It has been used in LSMs such as CLM, JULES,

1167 Noah-MP, CSLM and ISBA-SURFEX amongst others. Some LSMs only require information on the soil 1168 moisture distribution such as CABLE. O ORCHIDEE does not use the concept of F_{sat} but introduces the 1169 notion of a ponded fraction which serves the opposite of F_{sat} . Instead of increasing runoff, it does 1170 enhance infiltration since it allows the latter to develop over several time steps. JSBACH uses the Arno-1171 Scheme to calculate surface runoff and infiltration and uses soil water capacity to determine F_{sat} . The 1172 equations used calculate F_{sat} are listed in Table 2 and a more extensive description of the use F_{sat} in 1173 various LSMs, including the concepts used in the TOPMODEL are presented in Appendix A2.

LSM	Distribution of soil moisture	Distribution of precipitation	Distribution of Ks	Saturated fraction of grid cell	Description/Formulation of grid-scale I max	Grid cell soil moisture variability Equation used	b-parameter
OLAM-SOIL	No	No	No	Ponding is permitted, and the hydraulic head at the bottom of the pond is the Dirichlet upper boundary condition for Richards Eqn. in the soil layers. Infiltration is the direct solution of Richards Eqn.	Homogeneous within grid box	N.A.	N.A.
ParFlow-CLM	No	No	No	No	No	N.A.	N.A.
ORCHIDEE rev4783	No	No	Exponential pdf	No F _{sot} , i.e. no saturation excess runoff; but ponding can occur because of infiltration- excess runoff (see A3.9)	Maximum infiltration rate not imposed per se in the model concept. It is the outcome Ks distribution and infiltration from top to bottom via a modified Green-Ampt model (see A2.6)	Not described for the horizontal variability	N.A.
Catchment land surface model (CLSM)	Amended TOPMODEL approach: Grid cell soil moisture variability is tied to the catchment water table depth distribution. Moisture distribution is shifted by root zone water in excess (or deficit) of equilibrium conditions.	No	No	Amended TOPMODEL approach-local water table depth <i>d</i> is related to local topographic index, mean topographic index and mean water table depth. Saturated fraction equals the fraction of d>0	Maximum infiltration rate not imposed per se in the model concept. It is a complex outcome of off-line Richards equation simulations, TOPMODEL formulations and the model's dynamically varying spatial moisture fields (see A2.7)	Amended TOPMODEL approach: Grid cell soil moisture variability is tied to the catchment water table depth distribution. Moisture distribution is shifted by root zone water in excess (or deficit) of equilibrium conditions.	N.A.
ISBA-SURFEX	Reflected power pdf, or TOPMODEL approach	No	No	Two options available: 1. F_{set} is based on a Topmodel type approach ~4/($D_{\pi} = (\theta_{max} - (\theta))(d_{\pi})$) 2. Arno scheme following Dumenil and Todini (1992)	see A2.7	reflected power density function	Can be set to value 0.2 or 0.5 depending on model application
Noah-MP version 3.0	TOPMODEL approach	Exponential pdf	No	$F_{ext} = \left(1-F_{frx}\right)F_{max}\sigma^{-0.5f_d\left(F_{m1}-F_{loc1}\right)} + F_{frx}$	$P_d \frac{D_x(1-e^{-kdt\Delta z})}{P_d + D_x(1-e^{-kdt\Delta z})}$	N.A.	N.A.
JULES version 4.6	Modified TOPMODEL approach based on local topographic index $\lambda_{(pros)} = ln(T(z_{(prot)}) / T(z_P)) + \lambda_{in}$	No	No	$F_{car} = a_{c} exp\left(-c_{c} \lambda_{ack}\right)$	$(1 - F_{ext})\beta_{e}K_{e}$	Modified TOPMODEL approach based on local topographic index $\lambda_{local} = ln(T(z_{local}) / T(z_T)) + \lambda_m$	N.A.
CLM4.5	TOPMODEL approach	No	No		$(1 - F_{ext})K_a G_{lot}$	homogeneous within gridbox	N.A.
CABLE	Gamma pdf (Entekhabi and Eagleson, 1989) $f_{\rm e}(s)=\frac{1e^{\pi_{\rm e}}}{\Gamma(n_{\rm e})}s^{\alpha_{\rm B}-1}e^{-\lambda s}$	No	No	$F_{cat} = 1 - erf\left(\sqrt{\frac{\kappa_p}{\lambda_p}}\right)$	N.A.	Entekhabi and Eagleson (1989). $f_{\theta}(s) = \frac{\lambda_{\theta}^{\sigma_{\theta}}}{\Gamma(n_{\theta})} s^{\alpha_{\theta}-1} e^{-\lambda_{\theta}}$	N.A.
SSIB	No	Exponential pdf	No	$P_{aab} = \frac{1}{b_{SSW}} \log \left(\frac{R_{b} \Delta b}{P_{drop} \pi_{SSW}} \right) - \frac{c_{SSW}}{\pi_{SSW}}$	N.A.	Homogeneous within gridbox	constants based on different plant functional type (Xue et al., 1996)
CH-TESSEL / H-TESSEL	Reflected power pdf	No	No	$F_{\rm rat} = 1 - \left(1 - \frac{W}{W_{\rm cost}}\right)^{0/(b+1)}$	$(w_{\alpha\sigma} - w) + max \left(0, w_{\alpha\sigma} \left\{ \left(1 - \frac{W}{W_{\alpha\sigma}}\right)^{+} - \left(\frac{P_0 + P_d}{(b+1)W_{\alpha\sigma}}\right)^{+}\right\}^{+}\right)$	reflected power density function	$\max \left[\frac{q_{0} - \alpha_{00}}{\alpha_{0} + \alpha_{00}} \right]$
JSBACH version 3.0	Reflected power pdf	No	No	Arno scheme following Dümenil and Todini (1992)	For each timestep, infiltration is limited to the the difference between water holding capacity of the rootzone and the water content of the rootzone at the beginning of the timestep.	Homogeneous within gridbox	N.A.

1174

1175 **Table 2:** Overview of definition of parameters and properties affecting infiltration in the different LSM.

1176 **4.1.5.** Characterizing the Surface Saturated Hydraulic Conductivity, K_s

The saturated hydraulic conductivity, K_s , is a key soil hydraulic property that controls soil water fluxes and thus the infiltration of water in soils. However, K_s is a scale dependent parameter that strongly depends on the support size of the measurement (Ghanbarian et al., 2015), and it exhibits anisotropic behavior (Pachepsky and Hill, 2017). Despite its importance, point scale K_s is a parameter that is still very difficult to estimate from pedotransfer functions that are typically based on simple basic soil information such a soil texture and bulk density. However, this information only partly explains the variability observed in point scale K_s values. In the widely employed ROSETTA software (Schaap et al., 2001), that contains soil 1184 hydraulic properties and basic soil information for various soils and is used to estimate soil hydraulic 1185 properties, the logarithmicly transferred point scale K_s value is estimated with a coefficient of determination (R²) equal to 53.5 % when using bulk density, sand, silt, and clay percentages. Including soil 1186 1187 moisture content at field capacity and wilting point, the R^2 increased up to 64.7 %. The HYPRES database 1188 of soil hydraulic properties for European soils developed by Wösten et al. (1999) that contains information 1189 of 1136 horizons for hydraulic conductivity provided a PTF to estimate point scale K_s with an R^2 of 19 %. 1190 This function uses silt and clay content, bulk density, percentage organic matter, and whether the soil sample to derive the properties originated from the top soil or subsoil. A similar R^2 value was obtained by 1191 1192 Vereecken et al. (1990) using clay, sand and carbon content, as well as bulk density, for 127 undisturbed 1193 point scale samples. In order to further increase the prediction of point scale K_s structural properties in 1194 addition to currently used soil properties need to be considered (Vereecken et al., 2010).

1195 Currently, pedotransfer functions for point scale K_s are based on relatively small sample volumes. In 1196 addition, point scale saturated hydraulic conductivity shows a high spatial variability as it is not only 1197 controlled by textural properties but also by soil structural properties and by the management of soils 1198 (Strudley et al., 2008, Van Looy et al., 2017). Some of these aspects will be elaborated in more detail in 1199 Section 4.1.5.1. In this section, we review the different approaches that currently are being used in LSM 1200 to estimate K_s and to represent its spatial distribution at the grid scale.

1201 4.1.5.1. Spatial Distribution of K_s

Table 3 provides an overview of the approaches used to quantify grid scale K_s in 12 different LSMs. It must be stressed, that these estimations of grid scale K_s are based on PTFs (using the textural class as input for prediction), although the support scale for the development of these PTFs is in all cases the point scale.

1205 In all models studied in the analysis, K_s is considered horizontally uniform across the grid cell except for 1206 ORCHIDEE and ISBA-SURFEX. ORCHIDEE considers an exponential distribution of the infiltrability across 1207 the grid cell and with depth. Infiltrability is defined as the arithmetic mean of K_s in the deepest fully 1208 saturated layer and the hydraulic conductivity in the topmost unsaturated layer. ISBA-SURFEX also 1209 considers an exponential distribution of K_s within a grid cell but only for Hortonian runoff (Decharme and 1210 Douville, 2006). As already mentioned in Section 3, heterogeneous soil surfaces will generate runoff 1211 earlier on than homogeneous soil surfaces, which is partly caused by the heterogeneity in saturated 1212 hydraulic conductivity.

1213 With respect to the vertical heterogeneity, JSBACH, Noah-MP, and CABLE assume a constant K_s value with 1214 depth. CLSM, JULES, ISBA, ORCHIDEE, and OLAM-SOIL allow for both constant and depth variable Ks values. Vertical heterogeneity of K_s in CLM is derived directly from vertical heterogeneity in soil texture. 1215 1216 In ORCHIDEE, K_s decreases exponentially with depth using the K_s value defined at 30 cm depth as a 1217 reference value. The extent of the exponential decrease depends on an extinction factor. Furthermore, 1218 the K_s profile may be modified depending on root density. For example, CLSM differentiates between surface and root zone layer hydraulic properties (including K_s) in the Richards equation simulations that 1219 1220 are used in the derivation of time scale parameters of catchment-scale vertical moisture transfer. For 1221 subsurface runoff, CLSM uses a TOPMODEL based approach with a depth-dependent K_s. ISBA can consider 1222 up to 14 soil layers with a varying K_s value.

1223 **4.1.5.2.** Estimators for K_s

In all LSMs, the estimation of grid scale Ks is typically based on soil textural information, but using classical
PTFs developed for the point scale (details on these PTFs are provided in Appendix A4). These estimations
are often completed with specific estimation functions for organic rich soils (e.g., CLM 4.5, ISBA, JULES,
see details in Section 4.1.5.4 and Table 3).

1228 Rahmati et al. (2018) compared the K_s values for the point scale provided by Clapp and Hornberger (1978) 1229 with K_s estimates derived from field scale infiltration experiments using the global soil infiltration database 1230 SWIG. The K_s derived from these experiments did not show a dependence on soil textural properties. Only 1231 for sand and loamy sand the values of Clapp and Hornberger (1978) and the SWIG data were of the same 1232 order of magnitude. For all other textural classes SWIG values were larger by a factor two to a factor of 1233 more than one thousand. Weynants et al. (2009) pointed out that improved estimates of point scale K_s 1234 may be obtained by including structure-related information such as pedologic data and information about 1235 land use and crop management, which strongly affect surface soil properties, as a result of tillage, root 1236 growth, soil trampling by cattle etc. (see Section 6.1.).

1237 A notable advance is offred by OLAM-SOIL (Walko and Avissar, 2008b, Walko et al., 2000), which uses the 1238 pedotransfer functions developed by Weynants et al. (2009) or de Boer (2016) to estimate K_s . The PTFs of 1239 Weynants et al. (2009) are based on a dataset of 182 point scale soil samples of Belgian soils (Vereecken 1240 et al., 1990, Vereecken et al., 1989). They estimated the texture-dependent K_s value by extrapolating the 1241 unsaturated soil hydraulic conductivity data to saturation and then calculated the ratio between the 1242 textural dependent K_s and the measured K_s value, which was also available. This ratio is a measure for the effect of structural related properties on measured K_s and was shown to depend on the sand fraction in the soil.

Soil classes in CLSM are parameterized by Campbell (1974) equations and the corresponding hydraulic parameters including K_s are based on lookup tables for twelve different soil textural classes or using the PTFs of Wösten et al. (2001), which are both developed on point scale. Campbell's method used the Brooks-Corey parameterization of the soil water retention curve and a single point measurement of K at a given water content to calculate the complete hydraulic conductivity function.

- 1250 None of the models directly considers the effect of soil structure on saturated hydraulic conductivity. Only 1251 the OLAM-SOIL considers implicitly the impact of structural properties on K_s by linearly interpolating 1252 between the measured K_s value and the value of the hydraulic conductivity obtained at a pressure head 1253 of about -6 cm as proposed by Weynants et al. (2009). Based on the work of Jarvis (2007) this value was 1254 considered to delineate the saturation range that is controlled by structural properties.
- In JSBACH, K_s values are assigned to 11 textural classes based on data presented in Beringer et al. (2001).
 However, the origin of the tabulated K_s values that appear to be mean measured values for a specific
 textural class is not clear. Most likely, they were derived from the dataset of Clapp and Hornberger (1978).

1258 JULES uses sand and clay content to estimate the saturated hydraulic conductivity for the main soil 1259 column. Below the soil column is an additional `deep water store', within which K_s decreases exponentially 1260 with depth with a dampening factor set equal to 3 as proposed by Clark and Gedney (2008). K₃ values can 1261 also be defined for each soil layer and can account for the presence of soil organic matter (Chadburn et 1262 al., 2015a). Rahman and Rosolem (2017) incorporated the effect of preferential flow into JULES (but note 1263 that this has not yet been adopted in the current 'official' UKMO version of JULES), to allow simulation of 1264 highly fractured unsaturated Chalk soils. Their bulk conductivity (BC) model introduces only two additional 1265 parameters (namely the macroporosity factor and the soil wetness threshold parameter for fracture flow 1266 activation) and uses the saturated hydraulic conductivity from the chalk matrix. The BC model was 1267 implemented into JULES and applied to a study area encompassing the Kennet catchment in the southern 1268 UK and the model performance at the catchment scale was evaluated against independent data sets (e.g., 1269 runoff and latent heat flux). The results demonstrated that the inclusion of the BC model in JULES 1270 improved the simulations of land surface water and energy fluxes over the chalk-dominated Kennet 1271 catchment. This simple approach to account for soil structure has potential for large-scale land surface

modelling applications. ORCHIDEE uses VG soil parameters (K_s , n, α , θ_r , and θ_s) for each USDA class. In addition, a decay of K_s with depth is imposed (as also in JULES), as written in Section 4.1.1. With respect to the horizontal variability, ORCHIDEE uses an exponential PDF to describe horizontal heterogeneity.

1275 **4.1.5.3. Use of Soil Maps to Estimate K**s

1276 The previous section shows that the basic soil information that is used to derive the soil properties needed 1277 to estimate point scale K_s differs amongst the models. Importantly, each LSM, in particular when 1278 employed for weather forecasting or GCM studies, can use different soil maps to inform the model on soil 1279 hydraulic parameters (so called ancillary data). For example, CABLE uses the Zobler soil class information 1280 (Zobler, 1986). The version used by Decker (2015) uses the soil texture from the Harmonized World Soil 1281 Database (FAO, 2009), and so does JULES. OLAM-SOIL uses the SoilGrids data published by Hengl et al. 1282 (2014) and Hengl et al. (2017) The SoilGrids databases provide information on basic soil properties at 1283 seven depths in the soil profile up to 2m. They also provide estimates of the depth to bedrock and the 1284 distribution of soil classes. The gridded predictions were based on approx. 150.000 soil profiles and 1285 remotely sensed data. The input data used to estimate the soil hydraulic properties by CLSM or ISBA-1286 SURFEX are obtained from the Harmonized World Soil Database version 1.21 (HWSD1.21) and the State 1287 Soil Geographic (STATSGO2) project (de Lannoy et al., 2014). PARFLOW-CLM uses the UNESCO soil map 1288 of the world (FAO, 1988) to provide a global coverage of K_s values.

1289 The default soil texture map used in ORCHIDEE is the map presented by Zobler (1986) at 1° and it is used 1290 in the currently ongoing CMIP6 simulations. CMIP6 refers to the coupled model intercomparison project 1291 phase 6 that aims to address 1) how the Earth System is responding to forcing, 2) origins and 1292 consequences of systematic model biases and 3) the assessment of future climate change in the contect 1293 of internal climate variability, predictability and scenario uncertainty (Eyring et al., 2016). ORCHIDEE can 1294 also use two other soil texture maps. The first one is the map developed by Reynolds et al. (2000) at 1/12° 1295 and the second one is the surface SoilGrids maps at 1 km (Hengl et al., 2014). All these maps are used to 1296 define the dominant texture at the model resolution, using the USDA texture classification.

1297 CLM 4.5 uses the soil dataset produced by the Global Soil Data Task 2000 that comprises 4931 soil mapping
1298 units and contains the textural composition (sand and clay content). These data were used by Bonan et
1299 al. (2002b) to create a global soil map of mineral soil textural data. The global data on soil carbon content
1300 are obtained from ISRIC-WISE (Batjes, 2006), whereas the soil carbon content for the higher latitudes are
1301 obtained from the Northern Circumpolar Soil Carbon Database (Hugelius et al., 2013).

1302 **4.1.5.4.** *K*_s and Infiltration in Organic Soils

Four models listed in Table 3 adjust the calculation of K_s for soils rich in organic manner as these soils typically show higher K_s than mineral soils. Organic soils mostly refer to soils in the Northern latitude and tropical areas and include permafrost and peat soils. The first few centimeters of these soils typically have a soil organic carbon content of up to 100% (Lawrence and Slater, 2008). CLM 4.5 use the approach proposed by Lawrence and Slater (2008) to calculate K_s as

1308
$$K_{s,i} = (1 - f_{sc,i})K_{s,min,i} + f_{sc,i}K_{s,sc,i}$$
 [49]

where $f_{sc,i}$ is the soil carbon density of a soil normalized by the soil carbon density of peat in layer *I*, $K_{s,sc,i}$ is the saturated hydraulic conductivity [L T⁻¹] of the organic carbon fraction in layer *i*, $K_{s,min,i}$ is the saturated hydraulic conductivity of the mineral fraction [L T⁻¹], whereby $K_{s,min}$ is obtained from the point scale PTFs of Clapp and Hornberger (1978) and Cosby et al. (1984) and given by

1313
$$K_{s,min,i} = 0.0070556 \times 10^{-0.884 + 0.0153(\% sand)_i}$$
 [50]

1314 Values for $K_{s,sc}$ were given by Letts et al. (2000).

1315 In JULES and ISBA-SURFEX a geometric average of the point scale K_s is used to account for the effect of 1316 soil carbon following the approach of Chadburn et al. (2015b) and Decharme et al. (2016), respectively, 1317 with:

1318
$$K_s = K_{s,min}^{(1-f_{sc})} \times K_{s,sc}^{f_{sc}}$$
 [51]

For CLM 4.5, soil organic matter data are obtained from the Harmonized World Soil Database, except for the northern high latitudes which come from the Northern Circumpolar Soil Carbon Database (Hugelius et al., 2013). In ISBA, the soil organic carbon content is determinated from two soil horizons (0-30cm and 30-100cm) of the HWSD1.21.

1323 In JSBACH three additional classes are added to the 11 soil textural classes, namely peat, moss, and lichen, 1324 each with an average value of K_s according to Beringer et al. (2001).

In CLSM, soils are stratified into four levels of organic carbon content (de Lannoy et al., 2014), with the
 highest one (>8.72% C, i.e. >15% organic matter) representing peat. Peat parameters were taken from the
 point scale information provided by Wösten et al. (2001) that represent highly decomposed peat. In a

- 1328 recently developed peatland module for CLSM, parameters and model structure were further revised, i.a.
- 1329 accounting for the high macropore fraction of undecomposed peat by allowing direct infiltration to the
- 1330 water table when the top soil layer becomes saturated, i.e. effectively turning off the Hortonian runoff
- 1331 mechanism over peatlands (Bechtold et al., under review).

LSM	PTF to estimate for grid-scale K _s	Underlying soil maps to provide coverage of K _s	Use of soil structural information	K _s constant in grid cell	Variation of K _s with depth
OLAM-SOIL	Weynants et al. (2009) or de Boer (2016)	Soil Grids (Hengl et al., 2014)	Yes	Yes	Yes
ParFlow-CLM	Schaap and Leij (1998) for the first 10 soil layers and Gleeson et al. (2011) for deeper layers	FAO (1988) and Gleeson et al. (2011)	No	Yes	Yes
ORCHIDEE rev4783	lookup tables for van Genuchten soil parameters for each USDA class	Zobler (1986) at 1° is the default soil texture map, but other soil maps can be used alternatively: Reynolds et al. (2000) at 1/12° and the SoilGrids maps at 1km (Hengl et al., 2014)	No	No ^b	Yes
Catchment land surface model (CLSM)	Campbell (1974) or Woesten et al. (2001)	Harmonized World Soil Database version 1.21 (HWSD1.21) and the State Soil Geographic (STATSGO2 project) (De Lannoy et al. 2014).	No	Yes	Yes
ISBA-SURFEX	from Clapp and Hornberger (1978) or Cosby et al. (1984) (optional) ; for organic soils (Decharme et al., 2016)	Harmonized World Soil Database (HWSD; http://webarchive.iiasa.ac.at/ Research/LUC/External-World-soil-database/HTML/), (FAO/IIASA/ISRIC/ISSCAS/JRC, 2012) at a 1 km resolution from the Food and Agricultural Organization (FAO/IIASA/ISRIC/ISSCAS/JRC, 2012).	No	Yes	Yes
Noah-MP version 3.0	from Clapp and Hornberger (1978)	Harmonized World Soil Database (FAO, 2009) or Milovac et al. (2014)	No	Yes	No
JULES version 4.6	from Clark and Gedney (2008); for organic soils Chadburn et al. (2015)	The default configurations of JULES use soil ancillaries based on sand/silt/clay fractions from the harmonised world soil database (HWSD), using function of Cosby et al 1984.	No	Yes	Yes
CLM4.5	from Clapp and Hornberger (1978) and Cosby (1984), for organic soils Lawrence and Slater (2008)	Based on IGBP soil data set for mineral soils (IGBP, 2000), with organic soil described from ISRIC-WISE (Batjes, 2006) and the Northern Circumpolar Soil Carbon Database (Hugelius et al., 2013) ^a	No	Yes	Yes
CABLE	same as horizontal	CABLE rev 2.0 uses the Zobler soil class information [Zobler, 1986, 1999]. Decker [2015] uses sand/clay/silt fractions from the Harmonized World Soil Database [FAO, 2009], calculating soil properties from the textures as in CABLE rev 2.0 from Zobler [1986].	No	Yes	No
SSiB	from Clapp and Hornberger (1978) and Sellers et al. (1986)	Harmonized World Soil Database v.1.1 (FAO et al., 2009)	No	Yes	No
CH-TESSEL	Based on tabulated values for 7 textural classes including organic soils (Balsam et al., 2009)	FAO (2003) soil texture map	No	Yes	yes
JSBACH version 3.0	from Beringer et al. (2001)	Based on an improved FAO soil type dataset (Hagemann and Stacke, 2015)	No	Yes	No

^a The International Geosphere-Biosphere Programme (IGBP) soil dataset (Global Soil Data Task 2000) of 4931 soil mapping units and their sand and clay content for each soil layer were used to create a mineral soil texture dataset (Bonan et al. 2002b). Soil organic matter data is merged from two sources. The majority of the globe is from ISRIC-WISE (Batjes, 2006). The high latitudes come from the 0.250 version of the ^b based on exponential pdf (see Table 2 and A2.6)

1333

Table 3: Overview of approaches used for the spatial distribution of saturated hydraulic conductivity, K_s in the LSMs. References for Table 3: Weynants
et al. (2009), de Boer (2016), Hengl et al. (2014), Schaap and Leij (1998), Gleeson et al. (2011), FAO (1988), Zobler (1986), Reynolds et al. (2000), Campbell (1974), Wösten et al.
(2001), de Lannoy et al. (2014), Clapp and Hornberger (1978), Cosby et al. (1984), Decharme et al. (2016), FAO (2009), Milovac et al. (2014), Clark and Gedney (2008), Chadburn
et al. (2015b), Lawrence and Slater (2008), Batjes (2006), Hugelius et al. (2013), Zobler (1999), Decker (2015), Sellers et al. (1986), FAO (2003), Beringer et al. (2001), Hagemann
and Stacke (2015), IGBP (2000), Bonan et al. (2002a), Batjes (2006).

1339 **4.2. Numerical Treatment of Infiltration in LSM**

The precipitation simulated in LSMs either infiltrates into the soil or becomes runoff when the soil is saturated (Dunne overland flow) or if the precipitation rate exceeds the infiltration capacity of the soil (Hortonian runoff). As have been discussed above, various modeling approaches have been developed to describe infiltration and transition to surface runoff. In the following, we provide an overview of the numerical treatments used by the LSMs listed in Table 1.

1345 The version of ORCHIDEE described here (Ducharne et al., 2017) solves water infiltration and 1346 redistribution based on the diffusivity form of the Richards equation, using an 11-layer vertical 1347 discretization (de Rosnay et al., 2002). Since d'Orgeval et al. (2008), point (profile) scale infiltration is no 1348 longer calculated based on the Richards equation, instead, it invokes a piston-like wetting front inspired 1349 by the Green and Ampt (1911) formulation to simplify the boundary conditions under time-varying rainfall 1350 rates and soil moisture profiles. In ORCHIDEE, the speed of the wetting front propagation is simplified in 1351 two ways, which both tend to reduce infiltration compared to the classical Green and Ampt formulation: 1352 (i) the suction at the front is neglected, (ii) the hydraulic conductivity at the wetting front is not the soil K_s , but an arithmetic mean of K_s in the lowest fully saturated layer and $K(\theta)$ in the topmost unsaturated 1353 1354 layer (the resulting value is termed K_i). An iterative procedure is used to account for saturation of a soil 1355 layer after the other, and infiltration-excess (Hortonian) runoff results when the rainfall rate cannot 1356 infiltrate over a single ORCHIDEE time step of 30 minutes. In this framework, infiltrability depends on the 1357 profiles of K_s and $K_{(\theta)}$, which itself depends on K_s and θ based on the Mualem-van Genuchten model (Eq. 1358 [7] and [8]). The value of K_s at 30 cm depth is taken from Carsel and Parrish (1988) for the 12 USDA soil 1359 textural classes, but K_s exponentially decreases with depth following Beven and Kirkby (1979).

1360 In the original JULES version listed in Table 1, soil water fluxes are calculated by numerically solving the 1361 diffusivity form of the Richards equation, for the soil water content increment $\Delta \theta$, where $K(\theta)$ and $h(\theta)$ 1362 are given by either Brooks Corey (Eqs [4] – [6]) or van Genuchten (Eqs [7] and [8]) parametric models. The 1363 choice of parametric model is set by the user. Note that currently the JULES van Genuchten scheme uses 1364 parameters (h_c and n_{vq}) that are directly derived from the Brooks Corey soil ancillary parameters as used 1365 for the Cosby et al. (1984) $K(\theta)$ and $h(\theta)$ equations, rather than employing van Genuchten-specific PTFs 1366 given by Wösten et al. (1999), for example. The numerical scheme uses an implicit 'forward timestep 1367 weighting' for numerical stability, in which the water fluxes are first calculated as a first order finite 1368 difference scheme using Eq. [3], but then the moisture increments are recalculated with K and h given by 1369 the water contents after the timestep, effectively solving Eq. [52] (see Best et al., 2011 for detail):

1370

1371
$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z} \left(K(\theta + \delta\theta) \left(\frac{\partial h(\theta + \delta\theta)}{\partial z} + 1 \right) \right)$$
[52]

1372

The vertical discretisation in JULES is flexible and set by the user. For the standard operational configurations and current Earth System Model only four soil layers are used, with thicknesses of 0.1, 0.25, 0.65, and 2 m. For greater numerical accuracy, a finer discretisation has been applied (e.g., Chadburn et al., 2015b). Model time stepping in JULES is typically less than an hour but set also by the user. Recently, Haverd et al. (2016) and Cuntz and Haverd (2018) implemented a new soil (Haverd and Cuntz, 2010a) and snow model with physically accurate freeze-thaw processes within CABLE, which solved the Richards equation in the mixed form.

In JSBach (Hagemann and Stacke, 2015, Roeckner et al., 2003) the diffusive form of Richards equation is used with hourly model time stepping. The soil profile is disretized in the first compartment with 6.5 cm layer thickness and vertical infiltration is calculated based on the ARNO scheme according to Dümenil and Todini (1992), whereby water will infiltrate while precipitation is below the difference between local storage capacity and the initial water content within the root zone. In JSBach no ponding is allowed and the lower boundary has no impact on the infiltration rate.

1386 In SSiB (Sun and Xue, 2001a, Xue et al., 1991, Zhan et al., 2003) the water flow is solved by the diffusivity 1387 form of the Richards equation, whereby the soil is discretized non-uniformely with smaller layer 1388 thicknesses close to the surface (upper layer = 1.75 cm). Time stepping is less than an hour and runoff will 1389 occur if precipitation exceeds the saturated hydraulic conductivity, K_s . No ponding of water is allowed at 1390 the soil surface.

Noah-MP (Niu et al., 2011b, Schaake et al., 1996), JULES (Best et al., 2011), and CABLE (Decker, 2015, Kowalczyk et al., 2013, Kowalczyk et al., 2006b) also solve the Richards equation in its diffisivity form and none of these models calculate the infiltration rate directly from Richards equation. Vertical discretization varies between 2.2 cm (CABLE) to 10 cm (Noah-MP and JULES) for the upper layer and time stepping is less than a day for all models (see Table 1). No ponding is allowed for any of these three models and for Noah-MP and JULES the lower boundary does not affect infiltration, whereas for CABLE the infiltration will be modified by changes in the soil moisture profile due to groundwater influence.

Another set of LSMs solve the Richards equation in its mixed form such as Parflow-CLM (Kollet and Maxwell, 2006, 2008b), OLAM-SOIL (Walko et al., 2000), and ISBA (Boone et al., 2000, Decharme and Douville, 2006), the Catchment-Land Surface Model (CLSM) (Ducharne et al., 2000, Koster et al., 2000), and CABLE enhanced by Haverd et al. (2016) and Cuntz and Haverd (2018). Because these models solve the Richards equation in the mixed form the infiltration rate can be directly computed from solving
Richards equation. Nevertheless, ponding is only allowed in OLAM-SOIL, Parflow-CLM, and enhanced
CABLE.

1405 In CLSM, infiltration rates are not solely an outcome of the Richards equation simulations. They are one 1406 component of an overall catchment-scale model concept with other processes affecting infiltration rates. 1407 CLSM uses a non-traditional framework that strongly emphasizes the subgrid horizontal variability of the 1408 land surface hydrological processes. The results of the one-dimensional Richards equation simulations are 1409 combined with TOPMODEL formulations that control the varying water table depth and moisture fields at 1410 the catchment scale. From this combination, time scale parameters of catchment-scale vertical moisture 1411 transfer are derived. It is to be emphasized that in this approach the spatial water table depth distribution 1412 is an important factor influencing catchment-scale infiltration rates.

1413 **5. Sensitivity of Infiltration-runoff Process to Model Parameters**

Most sensitivity studies that have been performed with LSM models with respect to infiltration-runoff processes have focused more on the analysis of runoff and river discharge (e.g., Huang et al., 2017, Materia et al., 2010, Zhang et al., 2016) and less on the sensitivity of the infiltration process to model parameters. In this section, we will review the results from sensitivity studies on LSMs that provide information on key parameters controlling infiltration processes and thus ultimately the whole water and energy balance.

1420 One of the first studies to analyze the sensitivity of LSM to infiltration processes was conducted by 1421 Dirmeyer and Zeng (1999). They analyzed the sensitivity of infiltration to the treatment of convective 1422 precipitation and the choices made with respect to the vertical resolution of the soil profile and soil 1423 properties. They found that the choice of the thickness of the surface soil layer impacts the simulation of 1424 the infiltration, with thinner surface layers causing infiltration excess to be more likely as the thinner 1425 surface layer has a much smaller capacity. Basic information about the impact of the vertical discretization 1426 of the hydrological components is also provided in this review in Section 2.4.4. Unfortunately, in most 1427 LSMs the discretization is predefined and often fairly coarse. In addition, Dirmeyer and Zeng (1999) found 1428 that a "realistic" distribution of convective rainfall in space and time at the grid cell scale is needed to 1429 adequately represent the infiltration, and thus, surface runoff. In addition, evaporation of intercepted 1430 canopy water will be overestimated if "unrealistic" distributions of convective rainfall will be assumed. 1431 They also analyzed in detail the impact of having a depth dependent soil porosity (here they used three 1432 layers for the SSiB model) with a higher porosity for shallow soil layers and lower porosity (more

1433 compaction) for deeper ones. By doing so, they modelled larger infiltration amounts and reduced
1434 gravitational drainage. Finally, thinner soil layers (2 instead of 5 cm) were found to generate more
1435 infiltration excess, i.e. higher surface runoff, during high insensitivity rainfall events and soil melt.

Soet et al. (2000) analyzed different conceptualizations of the land surface scheme and parameter values for three sites with contrasting soils and climate using the ECMWF TESSEL land surface model developed by Viterbo and Beljaars (1995). A sensitivity analysis, set up to explore the impact of using standard parameter values instead of site-specific ones, found that implementing site specific soil hydraulic properties had a significant effect on runoff and infiltration at all three sites. On the other hand, the use of standard soil parameters led to a systematic underestimation of evapotranspiration and biases in surface runoff that differed in sign for the three different locations.

1443 The sensitivity of the infiltration shape parameter b in the VIC model (see Section 4.1.1) as well as the 1444 exponent in the Brooks Corey equation (Eg. [4] - [6]) were found to be key for correct representation of 1445 the hydrological system and the partitioning of rainfall between infiltration and runoff under dry soil 1446 conditions (Demaria et al., 2007). Ducharne et al. (1998) found a similar sensitivity to the b parameter for 1447 the bucket model version of ORCHIDEE. On the other hand, the impact of these parameters on surface 1448 runoff generation and stream flow simulations in wet regions was not significant. Shi et al. (2014) analyzed 1449 the sensitivity of the catchment outlet discharge rate to soil properties in the Penn State model Flux PIHM 1450 and found an important impact of the van Genuchten parameters h_c and $n_{vq}\alpha$ and n (see Eq. [7] and [8]) 1451 on both discharge rate and soil water content. Runoff simulations of ten state-of-the-art hydrological and 1452 land surface models including H-TESSEL, JULES, and ORCHIDEE were compared by Beck et al. (2017) and 1453 they argued for the need to better calibrate, parametrize, and regionalize the parameters of these macro-1454 scale models. Most models were found to generate snowmelt runoff that occurred too early, either due 1455 to the underestimation of precipitation or incorrect description of input snowfall, snow physics, and 1456 meltwater infiltration into the soil (Bierkens, 2015). Getirana et al. (2014) calibrated river routing 1457 parameters and stated that one of the most important aspects to getting the runoff timing (by 1 or 2 1458 months!) and runoff volumes right was the specification of the soil water threshold when runoff occurs 1459 (using the Habets and Saulnier (2001) option for runoff in ISBA). They extended the study of (Getirana et 1460 al., 2017) to a large group of LSMs including those presented here (e.g., CLSM, ISBA, H-TESSEL, JULES, 1461 ORCHIDEE) and found that this was also the case for most of the other LSMs in the ALMIP2 ensemble 1462 analysis. In another study, Gudmundsson et al. (2012) compared nine large scale LSMs including H-1463 TESSEL/CH-TESSEL, JULES, and ORCHIDEE to predict observed runoff percentiles of 426 small catchments

1464 throughout Europe and found, that the differences in performance between the models became more 1465 pronounced for low runoff percentiles. They concluded that this might be explained by the uncertainty 1466 associated with the representation of hydrological processes, such as the depletion of soil moisture 1467 storage by rootwater uptake. It is likely that differences in the treatment of infiltration and calculation of 1468 hydraulic properties will also have played a role. The performance of three LSMs was analyzed by Sahoo 1469 et al. (2008), including HySSiB, Noah, and CLM and the authors found substantial differences in the 1470 prediction of surface and subsurface runoff for the Little River experimental watershed, Georgia (USA), 1471 which was caused by differences in the partitioning of the precipitation into infiltration, surface runoff, 1472 and evaporation. An extensive analysis was presented by Zhou et al. (2012) who compared a set of 14 1473 land surface models (including VISA, CABLE, ISBA, CLMTOP, and Noah) and six Budyko-type models against 1474 the observed mean annual runoff from 150 large basins. They showed that the LSM biases in the 1475 prediction of the simulated mean annual runoff were caused by errors in forcing data, model 1476 parameterizations, but also by structural model errors. The largest biases between the LSM estimates and 1477 observed runoff were found in regions with low mean annual runoff, which corresponds with the findings 1478 of Gudmundsson et al. (2012). Hogue et al. (2006) evaluated the model performance and parameter 1479 sensitivity for varying levels of land surface model complexity across four different biomes using five LSMs 1480 including Noah-MP. They found a large variability amongst porosity, saturated hydraulic conductivity, K_s, 1481 and the *b* parameter used in these models. Based on the impact of these parameters on the simulation 1482 results, the authors advocate either a rigorous calibration or the development and integration of 1483 improved vadose zone water flow models. Especially, calibration of these parameters at different 1484 experimental sites led to differences with respect to the standard values. A study in the same direction 1485 was performed by Cuntz et al. (2016) who analyzed the role of hard coded model parameters (i.e., 1486 providing the user with no option to change values) on the hydrological fluxes in Noah-MP. They found 1487 that the total runoff was sensitive to both plant and soil parameters (e.g., soil porosity), and that 1488 therefore, these parameters should be considered for calibration. They also stated, that surface runoff is 1489 affected by subsurface runoff, which is dependent on available soil water in the soil profile. Yang and Niu 1490 (2003) compared three different schemes of topography-based runoff production for the LSM VISA (which 1491 is based on the LSM of Bonan (1998) and analyzed their sensitivities to key parameters using two 1492 catchments. They found that the decay factor, f, which controls the timing and partitioning of subsurface 1493 runoff by rescaling the saturated hydraulic conductivity, K_s , with depth, is a highly important parameter 1494 controlling water table depth and the saturated fraction of the grid cell. Shellito et al. (2016) compared 1495 calibrated soil hydraulic parameters in Noah using in-situ soil moisture network data and surface soil

1496 moisture from SMOS satellite observations obtained from seven sites in the US. Most calibrated 1497 simulations lead to higher surface runoff than simulations based on hydraulic parameters estimated from 1498 textural information using a pedotransfer function. The calibrated soil hydraulic parameters included pore 1499 size distribution index, saturated soil water content, saturated hydraulic conductivity, K_s , and the 1500 saturated matric potential (or air entry value, h_c) in the Brooks-Corey equations (Eq. [4] – [6]). Finally, Yang 1501 et al. (2005) concluded that the characterization of the vertical soil hydraulic heterogeneity is highly 1502 important to correctly describe soil water and soil temperature at the land surface and thus indirectly 1503 infiltration and surface runoff. Based on numerical simulations and experimental data, they concluded 1504 that it was not possible to replace vertical soil heterogeneity by a homogeneous soil with effective 1505 parameters.

1506 In conclusion, there is relatively little information provided in literature on how well the infiltration 1507 process and the generation of Dunne or Hortonian overland flow are modelled using different LSMs, and 1508 which model parameters mostly impact the infiltration process. In addition, this literature review indicates 1509 that it is difficult to identify sources of errors in handling infiltration estimation due to the complexity and 1510 the different ways in which the infiltration proces is being described. One approach to address 1511 comparisons of different approaches was proposed by Clark et al. (2015) who advocated the development 1512 of models that include different paramterizations of the infiltration process so that parameters and 1513 parameterizations can be evaluated in a controlled manner.

1514 **6. Improving the Infiltration Process in LSMs**

1515 The balance between parametrization of complex heterogeneous soil structure and exogenic processes 1516 that affect infiltration with the operational performance to compute infiltration/runoff processes that are 1517 embedded within LSMs, requires an understanding towards the trade-off of adding more complex physics 1518 to describe the infiltration/runoff process and the reality of the technical aspects of computing land 1519 surface processes and the determination of related parameters. Also, infiltration/runoff are just two of 1520 many other processes impacting the land-atmosphere interaction. This section therefore, aims to provide 1521 an overview to contextualise the complexity of the derivation of soil hydraulic parameters, rather than to 1522 point out the shortcomings of LSMs in terms of modelling infiltration and runoff.

1523 In general, there are many soil characteristics broadly related to soil composition and structure (including 1524 macro- and biopores), and also to exogenic processes, including water repellency, wetting and drying, 1525 swelling and shrinkage, air entrapment, freeze/thaw, thermal gradients, impermeable layers, and

- anthropogenic perturbations (e.g., tillage, harvesting) that impact infiltration and runoff at the point scale(see Young and Crawford (2004) and Hannes et al. (2016), for example).
- Most of these are presently not considered in most hydrological and land surface models, or not in enough detail and there is only little ongoing work in this sense such as the implementation of soil structure in the OLAM-SOIL model (see Table 3) by the use of a dual porosity model. Unfortunately, the main challenge in implementing soil structure into the LSMs lies in the lack of PTFs considering e.g. soil structure explicitly and also the temporal change of soil structure.
- 1533 In the following, we provide an overview of these processes and features and discuss the impact on 1534 infiltration and runoff generation briefly.

1535 6.1. Soil Structure

1536 The physical soil structure is formed by the combination of the size, shape, and arrangement of voids and 1537 solids, which ultimately affect water infiltration and runoff, mainly through the soil hydraulic properties 1538 (water retention and hydraulic conductivity curves) that are part of most LSMs and hydrological models. 1539 In general, the amount of water that infiltrates into a soil is dependent on the available void space 1540 (represented by the model soil layer porosity), which is the cross-sectional area of flow. Greater soil 1541 aggregation and pore connectivity increase bypass or preferential flow, therefore, increasing the hydraulic 1542 conductivity and movement of water to deeper soil layers (e.g., Franzluebbers, 2002, Nissen and Wander, 1543 2003). However, the process has not been implemented in most LSMs (Le Vine et al., 2016), apart from 1544 the efforts described in Rahman and Rosolem (2017). The formation of aggregates and the stability of the 1545 intra-aggregate void spaces is dependent on the rearrangement, flocculation, and cementation of soil and 1546 is mediated by the soil organic carbon (SOC), soil biota, ionic bridging, soil clay content, and carbonates. 1547 Additionally, macro-organisms facilitate soil porosity, infiltration, and aggregate stability by ingestion of 1548 soil (Brown et al., 2000). Factors affecting soil aggregation are summarized in Fig. 7. Macropores, defined 1549 as large continuous openings formed by macro-organisms (e.g., earthworm burrows, old root channels) 1550 have also an important influence on infiltration and subsurface storm flows as reviewed by Beven and 1551 Germann (1982) and for snowmelt infiltration by Mohammed et al. (2018).



1552

1553

Figure 7: Factors affecting soil aggregation (modified after Bronick and Lal (2005)).

Growing vegetation modifies the soil matrix, affecting soil hydraulic conductivity and soil water storage. Hereby, roots alter the distribution of pore size and connectivity between pores as they push into the soil matrix, and they also release complex organic compounds into the soil (Bengough, 2012). The continuous network of branched roots that permeate the soil, with new roots frequently forming while old ones decay, causes hydrological processes to change. Root length distribution is a key property that controls connectivity and preferential flow pathways within the rooting zone and thus impacts infiltration (Lange et al., 2009).

6.2. Hysteresis in the Soil Water Retention Curve and Thermal Effects on Hydraulic Properties

1563 Many LSM models assume that the difference between the soil water retention behaviour between 1564 wetting and drying phases in unsaturated soils (hysteresis) can be ignored and that the soil can be 1565 considered as having one unique soil water retention curve, which is used to solve Richard's equation (Eq. 1566 [3]).

However, hysteresis can play a crucial role in the accurate description of the flow processes within a soil
profile (Glass et al., 1989, Hanks et al., 1969, Ibrahim and Brutsaert, 1968, Scott et al., 1983). Hysteresis is
a process that describes the non-identical nature of equilibrium soil water content in relationship to
matrix potential, during the wetting or drying phases. The relationship between actual soil water content
and matric potential can be obtained in desorption, i.e. drying of wet soils, or sorption, i.e. gradual wetting

of dry soil. The resulting desorption/sorption curves are generally not identical, because equilibrium soil water content is greater at a given suction in drying than during wetting. The relationship of actual water content and matrix potential has been extensively studied by Haines (1930), Everett (1955), Poulovassilis (1962), Topp (1971), Mualem (1974), Mualem and Dagan (1975), Parlange (1976), Hogarth et al. (1988), Nimmo (1992), Bachmann and van der Ploeg (2002), Huang et al. (2005), and Mualem and Beriozkin (2009).

Thermal gradients also induce significant changes in the estimated water fluxes as temperature affects soil hydraulic properties (Ben Neriah et al., 2014, Gardner, 1955, Grant and Bachmann, 2002, Grant and Salehzadeh, 1996, Hopmans and Dane, 1986, Nimmo and Miller, 1986, Parlange et al., 1998, Philip and de Vries, 1957, She and Sleep, 1998). For example, increasing water temperature decreases water viscosity, causing an increase in hydraulic conductivity (Levy et al., 1989), and thermal swelling of solid particles that change soil pore characteristics and the solid/liquid interface between soil particles (Gao and Shao, 2015).

The advancement of innovative modelling that includes the hysteretic nature of soil water retention curve was reviewed and further developed by Nuth and Laloui (2008) but it has to be mentioned that for large scale LSMs the inclusion of hysteretic complexity requires greater computing capability and the knowledge of input parameters from observations and databases, or availability of appropriate pedotransfer functions.

1589 **6.3. Soil Water Repellency**

1590 Soil water repellency (SWR) or hydrophobicity reduces the affinity of soils to infiltrating water such that 1591 they resist wetting for periods ranging from a few seconds to hours or even weeks (e.g., Doerr and 1592 Thomas, 2000, King, 1981). Additionally, soil water repellency is spatially and temporally very variable 1593 (Regalado and Ritter, 2008, Ritsema and Dekker, 1998, Täumer et al., 2005). SWR is mostly caused by the 1594 coating of the soil particles by hydrophobic substances, whereby different organic compounds derived 1595 from living or decomposing plants or microorganisms can be responsible for SWR. Soils below particular 1596 vegetation types (such as needle leaf trees), soils with higher soil carbon content, coarse textured soils, 1597 as well as areas with frequent wildfire are more prone to SWR compared to others. A review of factors 1598 affecting SWR is given by Doerr et al. (2000). As mentioned, SWR will reduce the soil infiltration capacity 1599 (e.g., Imeson et al., 1992, Van Dam et al., 1990), and therefore, will increase overland flow (e.g., Crockford 1600 et al., 1991, McGhie and Posner, 1981, Witter et al., 1991). Topsoil SWR may cause Hortonian overland 1601 flow (runoff) even at precipitation events with rates much smaller than saturated hydraulic conductivity.

1602 In LSMs where K_s is derived from pedotransfer functions, and where water repellency is not included, this 1603 may lead to ovestimation of infiltration for SWR prone soils. In some areas, water repellent layers underlie 1604 highly permeable hydrophilic surface layers, and here, the infiltrating water may pond above the water-1605 repellent layer and subsequently the infiltration water can be stored above this hydrophobic layer and be 1606 used for evapotranspiration.



1607

Figure 8: Schematic illustration of possible hydrological responses of the soil under wettable and water repellent soils, layer bounds, spatial variability of soil hydraulic properties, and macropore flow induced by soil fauna and vegetation. Or et al. classnotes with permission.

1611 This process can also cause saturated excess overland flow if the above permeable layer becomes fully 1612 saturated, can cause lateral water flow either through structural gaps or along the slope of the hydrophilic 1613 layer, or the water can move downwards through the hydrophilic layer along preferential flow paths 1614 (Doerr et al., 2000). A schematic illustration of the possible hydrological responses caused by top and subsoil hydrophobicity is provided in Fig. 8. According to our knowledge, SWR has not yet been implemented in any LSM.

1617 **6.4. Compaction, Swelling, and Shrinkage**

1618 Compaction is the process of reducing the volume of voids in a soil, mainly those filled with air, by packing 1619 the soil particles closer together. It can result from natural processes such as soil overburden or from 1620 anthropogenic causes, such as the use of cultivation machinery or cattle grazing. Compaction is often 1621 characterized by the increase of soil bulk density. This has often been considered as an appropriate 1622 independent variable to quantify the decrease in the soil saturated hydraulic conductivity (Ahuja et al., 1623 1989, Assouline and Or, 2008, Laliberte et al., 1966, Or et al., 2000) or the changes in the soil hydraulic 1624 functions (Ahuja et al., 1998, Assouline, 2006a, b, Stange and Horn, 2005) following compaction. These 1625 estimates can thus be applied to evaluate the impact of soil compaction on infiltration. Soil swelling during 1626 wetting and shrinking during drying induces dynamic changes in porosity with changing water content of 1627 the soil and changes in the hydraulic properties, which consequently affect infiltration (Giraldez and 1628 Sposito, 1985, Philip, 1970, Raats and Klute, 1969, Smiles, 1974, Sposito, 1975). In general, the 1629 macroporosity, and to a lesser extent the microporosity, of swelling and shrinking soils is affected by their 1630 shrinkage and swelling behaviour (Alaoui et al., 2011), whereby exactly these voids in the pore system are 1631 highly important for rapid water infiltration into the soil and the separation between infiltration and 1632 runoff. Electrolyte concentration of the applied water also can have a significant impact on soil hydraulic 1633 properties and on the infiltration process. The way the soil structure behaves to electrolyte concentration 1634 depends on pedogenic processes and the nature of the parent material. For example, a high proportion 1635 of sodium ions relative to other cations weaken the bonds between soil particles, decreasing hydraulic 1636 conductivity (Frenkel et al., 1978, McNeal and Coleman, 1966, Quirk, 1994, Rengasamy and Olsson, 1991). 1637 This process and its impacts on soil physical and chemical properties is described in several studies 1638 (Assouline and Narkis, 2011, Assouline et al., 2016, Bresler et al., 1982, Greene and Hairsine, 2004, Jury et 1639 al., 1991, Kim and Miller, 1996, Quirk and Schofield, 1955, Russo, 2005).

Additionally, expansive soils, including peat, can adsorb large quantities of water during rainfall and therefore, reduce surface runoff. According to the USDA soil classification clayey soils with clay content >30% (often Vertisols) cover around 320 million ha globally and are sensitive to swelling and shrinkage (Dinka and Lascono, 2012). Several studies have looked at the dynamics of shrinking and swelling and associated crack changes for the purpose of improving hydrological models (e.g., Arnold et al., 2005, Bronswijk, 1991, Kishné et al., 2010), but none for LSMs. An extensive review of these models is provided

by Adem and Vanapalli (2015). Unfortunately, the shrink-swell properties of the Vertisols vary also as a function of soil properties, climate, topography, vegetation, cropping management, and management practices (Davidson and Page, 1956, Lin et al., 1998, Thomas et al., 2000, Vaught et al., 2006), which complicates the representation in hydrological and land surface models.

1650 **6.5. Freeze and Thaw**

1651 Many soils at higher elevation or latitudes freeze and thaw seasonally, impacting the soil physical 1652 properties, and therefore, affect the water movement in the landscape substantially. The main effect of 1653 freeze-thaw cycles (FTC) on soil properties lies in the impact on the soil structure, which, as shown earlier, 1654 regulates infiltration and runoff to a large extent (e.g., Chamberlain and Gow, 1979, Fouli et al., 2013, Qi 1655 et al., 2006). Freezing and thawing processes induce uneven stress within the soil but the conclusions in 1656 the literature about the effects on soil structure and water flow are not unanimous. There are indications 1657 that FTC decreases soil stability (Edwards, 1991, Kværnø and Øygarden, 2006), whereas Lehrsch (1998), 1658 Lehrsch et al. (1991), and Park et al. (2011) observed increasing stability after a few FTCs, while an 1659 increased number of FTCs caused a decrease in soil stability, leading to changes in soil hydraulic 1660 parameters over time. On the other hand, there seems to be more consensus that the effect of FTC on 1661 clayey soils is much larger than on coarse textured soils (Bisal and Nielsen, 1967, Kværnø and Øygarden, 1662 2006). Unger (1991) additionally stated that FTC decrease soil bulk density.

1663 It is also known that the hydraulic conductivity of frozen soil decreases rapidly as the temperatures fall 1664 (Williams and Burt, 1974), and some models do take this into account (e.g., CLM, Noah-MP, SSiB, SURFEX, 1665 CABLE, OLAM-SOIL, ORCHIDEE). Additionally, even water in the liquid phase is impacted by temperature 1666 changes as the viscosity of the pore water increases significantly with decreasing soil temperatures (Hillel, 1667 1998) leading to lower fluidity and water percolation even before freezing. Finally, if the freezing front is 1668 near the soil surface, ponding is likely to occur at the soil surface after a precipitation event, resulting in 1669 runoff, because the amount of liquid water-filled pathway has reduced. Most LSMs take this effect into 1670 account. Also, as the freezing front moves down the soil profile, soil water will migrate towards the 1671 freezing front, leaving a drier soil behind, resulting in a larger matric potential gradient pulling the water 1672 towards the freezing front (Jame, 1977). Even though some LSMs account for the direct impact of freezing 1673 on the saturated hydraulic conductivity, $K_{\rm s}$, temporal changes on the hydraulic parameters due to 1674 structural changes induced by FTC are not implemented yet. This might be problematic for regions where 1675 FTC might become more frequent in future climate as stated by Eigenbrod (1996).

1676 6.6. Impermeable Soil Layers

1677 Impermeable layers, or more precisely soil horizons with extremely low saturated hydraulic conductivity, 1678 frequently occur in natural or managed soils. Often these layers are denoted as hardpans, hard layers, or 1679 compacted horizons either located at the surface or subsurface (Busscher, 2011). These layers can be 1680 caused by traffic, tillage practices, trampling of livestock, or soil forming properties that result in layers 1681 with high density or cemented soil particles (Hamza and Anderson, 2005, Silva et al., 2000). For example, 1682 the extent of compacted soil is estimated worldwide at 68 million hectares of land from vehicular traffic 1683 alone (Flowers and Lal, 1998). Some of these compacted or extremely dense soil layers are relatively thin, 1684 and are therefore, often neglected in soil maps at coarser scales. Additionally, changes in the saturated 1685 hydraulic conductivity due to soil compaction is often not accounted for in pedotransfer functions, if bulk 1686 density is not used for the prediction of the hydraulic parameters (Van Looy et al., 2017). Nevertheless, 1687 these layers are of utmost importance because they control the infiltration of water into the soil, and its 1688 redistribution to greater depth. In general, presence of impermeable soil layers will lead to the same 1689 hydrological response as shown for the hydrophobic layers depicted in Fig. 8, generating more overland 1690 flow (runoff) and sub-surface storm events.

1691 Impermeable layers complicate the naturally occurring soil vertical heterogeneity, where generally 1692 successive distinct layers of soil with different hydraulic properties occur. Several studies have proposed 1693 solutions for infiltration in layered soil systems (Childs and Bybordi, 1969, Colman and Bodman, 1945, 1694 Hanks and Bowers, 1962, Miller and Gardner, 1962, Philip, 1967, Raats, 1973, Warrick and Jim Yeh, 1990, 1695 Zaslavsky, 1964). Chu and Marino (2005) presented a solution for determining ponding conditions and 1696 simulating infiltration into a layered soil profile based on the Green and Ampt approach for unsteady 1697 rainfall. Beven (1984) and Selker et al. (1999) also extended the Green and Ampt model for infiltration 1698 into soil profiles where pore size varied with depth. A review of the applications of the Green and Ampt 1699 model to vertically heterogeneous conditions was provided by Kale and Sahoo (2011).

A special case of layered soil profile occurs when a seal layer or crust develops on the soil surface, resulting from the destructive action of raindrop impacts on the soil, which alters the soil structure and soil hydraulic properties, especially the saturated hydraulic conductivity, *K*_s. This process and its impacts on physical and chemical properties is described by Quirk and Schofield (1955), Bresler et al. (1982), Jury et al. (1991), Kim and Miller (1996), Greene and Hairsine (2004), Russo (2005), and Assouline et al. (2015). A review of the approaches proposed to model infiltration into sealed (or crusted) soils can be found in Mualem and Assouline (1992), Mualem and Assouline (1996), and Assouline (2004). The direct effect of 1707 the presence of the impeding seal layer at the soil surface is to reduce ponding time and infiltration rate 1708 during rainfall (Römkens et al., 1986, Romkens et al., 1986). Hillel and Gardner (1969, 1970) first addressed 1709 the problem of infiltration in the case of sealed soils. They presumed that a sealed soil can be modelled 1710 as a uniform soil profile capped with a saturated thin layer of low permeability with constant prescribed 1711 physical properties such as the saturated hydraulic conductivity. Their simplified solution was based on 1712 the Green and Ampt model, assuming a constant water content (or suction) at the interface between the 1713 seal and the soil beneath. It was further applied in different studies (Ahuja, 1974, Ahuja, 1983, Moore, 1714 1981a, Parlange et al., 1984). Variations and extensions of this basic approach included the simulation of 1715 infiltration with time-dependent seal hydraulic conductivity functions (Ahuja, 1983, Brakensiek and Rawls, 1716 1983, Chu et al., 1986, Farrell and Larson, 1972, Moore, 1981b, Vandervaere et al., 1998, Whisler et al., 1717 1979). An additional conceptual model, based on the model of Corradini et al. (1997), was suggested by 1718 Smith et al. (1999). Römkens and Prasad (1992) applied the solution of Prasad and Römkens (1982) based 1719 on the spectral series approach to solve the infiltration equation in soils topped by a constant or transient 1720 crust.







Figure 9: The impact of soil surface sealing on infiltration.

1723 Here, it has to be noted that in all these studies the hydraulic properties of the seal layer were arbitrarily 1724 chosen. Mualem and Assouline (1989) as well as Baumhardt et al. (1990) have addressed the problem of 1725 infiltration into sealed and sealing soils by attributing to the seal layer hydraulic functions that evolved 1726 from those of the undisturbed soil, and that were related to the specific rainfall kinetic energy and 1727 intensity involved in the seal formation. The impact of soil surface sealing on infiltration is illustrated in 1728 Fig. 9, where it is depicted that soil surface sealing reduces the ponding time and the infiltration rates into 1729 the soil profile, including the final quasi-steady rate. As a result, much more runoff is formed by a given 1730 rainfall event when the soil surface sealing is accounted for.

1731 **6.7. Instability of Different Flow Regimes**

1732 Wetting front instability occurring under certain flow regimes can also affect significantly the infiltration 1733 process (DiCarlo, 2004, Jury et al., 2003, Or, 2008, Parlange and Hill, 1976, Philip, 1975, Raats, 1973). 1734 Wetting front instability refers to a splitting up of the infiltration front into several fingers along which 1735 water is transported downward rapidly. Since a part of the soil pore volume is bypassed by the infiltration 1736 through fingers, wetting front instability leads to considerably deeper infiltration than in case of stable 1737 wetting fronts. Raats (1973) explained that an increase of soil water pressure with depth above the 1738 wetting front in general leads to instabilities of the wetting front. Entrapment of air, the presence of layers 1739 with higher water entry values, water repellency, but also the reversal of pressure gradients during 1740 redistribution just after infiltration at the soil surface ceased can cause such an increase in pressure above 1741 the wetting front that leads to unstable wetting fronts (Wang et al., 1998, Wang et al., 2003a, Wang et 1742 al., 2003b). Another process, which orginates at the pore scale and which can explain the persistence of 1743 individual fingers due to pressure increase or pressure overshoot above the wetting front of a single finger 1744 is the dynamic pressure-water content relation that results from a rapid filling of larger pores and a 1745 subsequent redistribution (DiCarlo, 2013).

1746 **6.8. Solution of Numerical Issues**

Rainfall of different rainfall intensity also affects infiltration depths and runoff ratios (Frauenfeld and
Truman, 2004). For example, varying intensity rainfall simulations yield larger runoff ratios and peak
runoff rates in comparison to uniform rainfall simulations (Dunkerley, 2012). Using Horton equations,
predicted runoff rates were significantly improved during intra-event time variation of fluctuating rainfall
simulations (Dunkerley, 2017).

1752 Conventional solution methods to the highly non-linear Richards' one-dimensional partial differential 1753 equation (PDE) equation used in LSMs inevitably lead to numerical and accuracy issues, which impact on 1754 their hydrological performance. LSMs may consider the implementation of alternative 1-D unsaturated 1755 zone flow solution methods (such as those provided by Ogden et al. (2015). The Ogden Soil Moisture 1756 Velocity Equation (SMVE) approach uses the hodograph method to transform Richards equation into a 1757 differential equation for a velocity, and employs a discretisation of the resulting equation in the form of 1758 'bins' containing values of the water content. The scheme is computationally efficient, although the 1759 explicit time steps are limited by stability considerations because there are no convergence limits as 1760 imposed by implicit schemes. Ogden et al. (2015) consider the transport of three regimes of soil water in 1761 detail, namely infiltration, wetting fronts disconnected from the surface, and groundwater recharge. The 1762 SMVE method offers accuracy comparable to, or in some cases exceeding, that of the numerical solution 1763 of the Richards partial differential equation method, but without the numerical complexity and in a form 1764 that is robust, continuous, and suitable for use in models of coupled climate and hydrology at a range of 1765 scales.

1766 **7. Summary and Conclusion**

1767 Infiltration processes are at the core of land surface models, representing the complex and highly dynamic 1768 coupling between precipitation and land surface properties where soil, vegetation, initial soil conditions, 1769 and topography interact. Although the formulation of infiltration representation for the soil profile scale 1770 is well established and tested by the soil physical community, there are still issues that need resolving 1771 with regards to the parameterisation of infiltration in LSMs. In particular, the extension of the concepts 1772 to the catchment and global grid cell scales remains challenging and is in some cases tentative, and with 1773 various different solutions that are currently in use. In this perspective, we reviewed and analyzed the 1774 different approaches used in current land surface models to predict soil infiltration processes. Specific 1775 attention was given to the underlying physical principles and concepts used to predict infiltration at the 1776 point and grid scale and the approaches used to describe spatial heterogeneity and upscaling of key 1777 parameters controlling the infiltration process in LSMs. We identified several topics and processes that 1778 warrant further attention in advancing the prediction of infiltration processes.

First, there is the prediction of saturated hydraulic conductivity, a key parameter in describing infiltration.
Currently, *K_s* estimates in LSMs are derived from pedotransfer functions that are typically based on the
textural composition of soils but do not consider the impact of soil structure on the infiltration process in
general. Recently, Rahmati et al. (2018) published a global database of infiltration measurements that

1783 clearly shows that K_s derived from field experiments can not be predicted from soil texture alone. 1784 Therefore, research needs to be directed towards the development of pedotransfer functions that consider the effect of structural properties on K e.g. using land use and tillage treatment as proxies (Jorda 1785 1786 et al., 2015). This might be even more important as a recent study of (Hirmas et al., 2018) indictates that 1787 drier climates induce the formation of greater soil macroporosity than do more humid ones, and that such 1788 climate-induced changes occur over shorter timescales than have previously been considered. Translation 1789 of the effects of these different, largely exogenic, processes to time-varying hydraulic properties (currently 1790 hydraulic properties in LSMs are kept constant in time) is one of the greatest challenges in current land 1791 surface modelling. For example, the increase of high-frequency rainfall event under future climate 1792 conditions will make crust-formation for certain soil types more likely, which will cause a decrease in 1793 infiltration and increase in surface runoff. Ignoring these aspects will add further uncertainties to 1794 predictions of future land-atmosphere interactions. This issue needs to be addressed urgently and in a 1795 coherent fashion whereby other soil properties (e.g. thermal properties) and vegetation parameters that 1796 depend on, or affect, soil properties (such as rooting depth) are changed concurrently.

Additionally, numerical simulations are needed to quantify the effect of K_s estimates considering the role
of soil structure on the energy, water, and matter cycles.

1799 Secondly, due to the availability of spatially highly resolved soil map information at the global scale with 1800 a spatial resolution of 250 m or even less, quantification of the subgrid variability is now within reach. The 1801 use of this information in combination with pedotransfer functions allows direct estimation of b, a lumped 1802 parameter used in several LSMs to describe the spatial variability of infiltration capacity. In addition, this 1803 highly resolved spatial information can be used to derive effective soil hydraulic parameters such as the 1804 Mualem van Genuchten parameters, which are used in the solution of Richards equation. The increasing 1805 availability of highly resolved spatial data poses questions on how to effectively and efficiently represent 1806 subgrid soil and landscape information in LSMs. The strengths and weaknesses as well as the validity and 1807 applicability of the methods presented in this review paper with respect to modelling land surface 1808 processes at the continental and global scale still has not been addressed.

The requirement to correctly represent Hortonian infiltration but also redistribution processes of water in the subsurface (e.g., due to root water uptake or capillary rise) is best fulfilled by using a Richardsequation based approach. Stochastic analyses of water flow in spatially heterogeneous soil fields (Mantoglou and Gelhar, 1987a, Mantoglou and Gelhar, 1987b, Vereecken et al., 2007b) have shown that the upscaled Richards equation at the field or larger scale has a form similar to the local scale equation.
1814 However, the spatial variability of soil hydraulic properties introduces a hysteretic behaviour of the larger 1815 scale system, as the effective hydraulic conductivity is a function of the hydraulic gradient and of its history 1816 reflecting non-equilibrium conditions. How far this non-equilibrium behaviour is relevant for grid scale 1817 infiltration processes needs to be further studied. The definition of the effective parameters in the 1818 upscaled Richards equation, however, requires detailed knowledge of the spatial statistics of local scale 1819 hydraulic parameters. The availability of highly resolved soil maps in combination with pedotransfer 1820 functions opens up new opportunities to define subgrid variability of hydraulic parameters and thus to 1821 quantify effective hydraulic parameters at the scale of LSMs. Also for heterogeneous porous media, the 1822 solution of the Richards equation for an infiltration problem remains stable (Egorov et al., 2003). To 1823 represent the impact of soil structure, macropores, cracks, or other well connected structures on water 1824 infiltration in soils, several modifications ranging from changing the typically used uni-modal pore size 1825 distribution to a dual or multimodal pore size distribution to introducing an extra flow equation that 1826 represents the infiltration in the macropre pore network and that is coupled with the flow equation in the 1827 soil matrix have been proposed (see reviews of Jarvis (2007) and Simunek et al. (2003). These well 1828 connected and highly conductive structures could also be represented in 3D Richards models (e.g., Vogel 1829 et al., 2006). But even for such media, the solution of the Richards equation leads eventually to relatively 1830 stable infiltration profiles that could be represented fairly well by an upscaled Richards equation with 1831 effective parameters (e.g., Schlüter et al., 2012). It must be noted, though that the local water fluxes above 1832 the infiltration front can be very heterogeneous (but the wetting front is relatively homogeneous). 1833 However, the Richards equation cannot reproduce unstable infiltration fronts that are observed at the 1834 local scale as a consequence of pore scale dynamic effects. Phenomena like finger development in gravity 1835 dominated flow, which can have an important impact on the vertical distribution of the infiltrated water 1836 and how it varies with infiltration rate at the soil surface, are therefore, not represented by the Richards 1837 equation. Several approaches to account for these dynamic and non-equilibrium processes by adding 1838 additonal terms to the continuum Richards equation have been proposed (Cueto-Felgueroso and Juanes, 1839 2009, DiCarlo, 2013, Eliassi and Glass, 2002). Although, these approaches describe experimentally 1840 observed non-uniform infiltration fronts, it still requires further investigation how the upscaled non-stable 1841 infiltration can be described by a continuum model and what its consequences are for the water 1842 distribution during an infiltration event at the LSM grid scale.

Also, correct representation of Hortonian infiltration requires consideration of vertical heterogeneity of
soil hydraulic parameters, a vertically variable discretization with the finest discretization near the surface,
and the use of a pressure head based Richards equation. Recently, LSMs such as Parflow/CLM, ISBA, CLSM,

and OLAM-SOIL have developed approaches that allow these requirements to be fullfiled. Introducing
similar approaches in other LSMs automatically avoids the need to define a maximum infiltration capacity
of soils leading to a more physically consistent description of infiltration.

1849 We observed a disparity between the approaches used at the field or small catchment scale, presented in 1850 Section 3, and the approaches applied at the grid scale in LSMs, presented in Section 4. This of course is a 1851 result of having two different scientific communities working predominantly at different spatial scales. 1852 The soil physics community mainly focuses on the field scale and typically uses semi-analytical solutions 1853 or full implementations of the Richards equation to explicitly solve for infiltration flux. This in general 1854 requires fine vertical discretization (~mm near the surface boundary) and short time steps (seconds) to 1855 calculate infiltration fluxes. Modelling of infiltration in LSMs is performed at much larger scale, which 1856 usually does not allow for a fine spatial and temporal discretization in order to keep the models 1857 computationally efficient. The majority of the LSM community has therefore taken the approach to 1858 parameterize the infiltration process at the land surface and use the Richards equation, mainly in the 1859 diffusive form, to redistribute infiltrated water in the soil profile. The common basis for both approaches 1860 is Richards equation, even though for different reasons. It is, however, the goal of this review to foster 1861 the cooperation and the exchange of ideas between the two communities. As a first step, the work of 1862 Montzka et al. (2017) provides a global concept of subgrid variability of soil hydraulic properties along the 1863 methods of similarity scaling. As the need increases to account for subgrid variability in LSMs, these above-1864 mentioned methods provide options for incorporating this uncertainty.

1865 Furthermore, there is a large diversity among the analyzed LSMs in estimating key properties such as soil 1866 moisture capacity and in the treatment of heterogeneity of soil moisture at the grid scale. In case of soil 1867 moisture heterogeneity three mathematical formulations have been used: i) reflection power distribution 1868 functions, ii) gamma distributions, and iii) exponential distributions with a variable number of parameters 1869 (two, three). In some cases LSMs also use different approaches to derive the saturated fraction (F_{sat}) of a 1870 grid cell, which is used to partition between Dunne saturation excess and Hortonian infiltration excess. Besides differences in concepts used to formulate the saturated fraction, there is a large divergence in the 1871 way the saturated fraction of the land surface within a pixel, F_{sat} , is being parameterized. 1872

Differences include whether or not groundwater depth is explicitly simulated, and if so, how; and the
treatment of the storage capacity of the soil between the land surface and the bedrock or groundwater
table depth.

1876 In addition, our analysis showed that basic soil information that is used to obtain spatial coverage of key 1877 soil hydraulic properties strongly differs between land surface models but also between the various 1878 version of one single LSM. The impact of using different spatial soil maps combined with the wide range 1879 of approaches used to estimate the saturated hydraulic conductivity, *K*_s, and other soil hydraulic 1880 properties is not yet known. Further research is needed in this direction to quantify the impact of this 1881 input variability.

Also, many LSMs use a prescribed parameterization of maximum infiltration capacity to partition precipitation between infiltrable water and runoff (exceptions being Parflow/CLM, ISBA-SURFEX, ORCHIDEE, CLSM, and OLAM-SOIL). These approaches have been heavily tuned by each LSM to ensure they fit with runoff observations. The lack of a general framework for this central hydrological process leaves a serious gap in the present LSM parameterizations and hinders simple and transparent updating of soil information when it becomes available.

1888 Moreover, re-infiltration, called runon is ignored in most LSMs; runoff production that occurs at sites 1889 where the infiltration capacity is exceeded may reinfiltrate in the grid cell due to soil and land surface 1890 heterogeneity, so that not all of the runoff that is generated at a grid cell needs to be routed out of the 1891 cell or to a receiving water body. A classic example is the runon in vegetation patches or bands(strips) in 1892 semi-arid regions (Assouline et al., 2015). Roots can increase the local infiltration capacity so that runoff 1893 from sealed non vegetated areas can infiltrate in vegetated areas (Nimmo et al., 2009). In addition, runon 1894 leads to a scaling behavior of rainfall runoff relations with generally less runoff produced at a larger scale 1895 than what would be derived from smaller scale rainfall-runoff relations. A crucial property that defines 1896 the rainfall-runoff relations at larger scales is the connectivity of regions that generate runoff (Herbst et 1897 al., 2006).

1898 Finally, several processes that control infiltration and thus impact the soil water balance, and ultimately 1899 the energy balance and related land-atmosphere interactions, at the grid cell scale require more attention. 1900 This includes the role of the vegetation in the infiltration process, the role of runoff-runon process at the 1901 grid cell scale and the dynamics of soil structural properties. Correct representation of the runoff-runon 1902 process will need spatially distributed information about parameters controlling Hortonian infiltration 1903 excess generation and the formulation and parameterization of redistribution mechanisms within the grid 1904 cell. The role of vegetation is related to the effect it exerts on the structural status of the vadose zone 1905 leading to soil properties that are changing over time. In addition, changes in land use and management 1906 may affect the structural status of the vadose zone and thus effect water infiltration in soils. One way

forward would be to develop pedotransfer functions that consider time dependent soil properties. This, however, requires a basic understanding on how vegetation and management practices change soil hydraulic properties of soils, suggesting the need for greater integration of soil physics, plant science and land management. There is increasing evidence that spatial variability in water infiltration may also be attributed to dynamics of vegetation-driven-spatial heterogeneity (Archer et al., 2013, Archer et al., 2012, Puigdefabregas, 2005) leading to increased infiltration capcity of soils. These processes that may lead to a decrease in Hortonian infiltration have not yet been introduced in land surface models.

1914 Currently, activities have been initiated between ISMC SoilMIP, and GEWEX (https://soil-1915 modeling.org/activities/events/the-gewex-soilwat-initiative-first-planning-workshop-for-scope-and-

interactions-advancing-integration-of-soil-and-subsurface-processes-in-climate-models) to advance the implementation of high quality soil information and the description of soil processes in LSMs. These improved LSMs, in turn, will feed into ESMs for global prediction and closure of water, energy, and carbon budgets. This review is a part of this initiative and one of the first outcomes of this joint activity based on a workshop held in Leipzig, Germany in 2016. Further activities are presently running such as the analysis of the effect of incorporating soil structure on the soil water balance of the terrestrial system and new ones are being initiated and developed.

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3079 List of Symbols

3080	a_s	fitting parameter for each grid box to estimate F_{sat} (JULES)
3081	a _{SSiB}	constant in Eq. [A54] (-)
3082	a _r	fitting parameter in CLSM
3083	b _r	fitting parameter in CLSM
3084	А	fraction of an area for which the soil moisture capacity is less than or equal to I (-)
3085	AC	steady state infiltration (LT ⁻¹)
3086	A_f	fitting parameter
3087	A_{gf}	grid box fraction of soil water capacity (-)
3088	A_1	fitting parameter (LT ⁻¹)
3089	b	parameter that reflects the grid cell heterogeneity (-)
3090	b _{SSiB}	constant in Eq. [A54] (-)
3091	b _{BC}	parameter in the Brooks Corey equation (Clapp and Hornberger, 1978) (-)
3092	В	potential infiltration rate shape parameter which is a measure for the spatial variability of the
3093		potential infiltration rate defined as the maximum infiltration rate of each point when the
3094		surface is ponded (Liang and Xie, 2001) (-)
3095	B'	parameter related to the BC exponent of the water retention characteristic (-)
3096	B_{TW}	exponent of the tension water capacity distribution curve (-)
3097	С	fraction of an area for which the potential infiltration rate is less than or equal to f (Liang and
3098		Xie, 2001) (-)
3099	С	water storage capacity at a certain location (L)
3100	C _{SSiB}	constant in Eq. [A54] (-)
3101	c_{max}	maximum water storage capacity (L),
3102	C _{ice}	ice impedance factor (-)
3103	Cs	fitting parameter for each grid box to estimate F_{sat} (JULES)
3104	C_v	tunable parameter (-)
3105	D_b	spatially averaged soil moisture storage deficit (-)
3106	D _{bmax}	maximum soil water storage (L)
3107	D_x	soil water storage (L)
3108	D_{θ}	average water table depth (L)
3109	D _{sm}	local soil moisture deficit (L)
3110	D_t	mean water storage deficit (L)
3111	D_{θ}	the amount of water stored between surface and groundwater (L)
3112	d _o	maximum local water deficit (L)
3113	\overline{d}	mean water table depth (L)
3114	dx	length of the grid cell in km (L)
3115	$\langle d_2 \rangle$	depth of the root zone (L)
3116	F _{sat}	saturated fraction of the catchment or grid cell in a LSM (-)
3117	F _{max}	fraction of pixels in a grid cell whose topographic index is larger than or equal to the grid cell
3118		mean topographic index (-)
3119	F _{frz}	fractional impermeable area as a function of soil ice content of the surface soil layer (-)
3120		cumulative distribution of mean infiltrability (ORCHIDEE)
3121	F(c)	standard reflected power cumulative distribution function of the spatial variation of the storage
3122		capacity, c
3123	$F_S(z^*)$	cumulative distribution function of the scaled infiltration capacity Eq. [47]
3124	f^*	infiltrability of the first soil layer (LT ⁻¹)

3125	f.	pdf of the respective variables
3126	f	point potential infiltration rate (LT ⁻¹)
3127	f_c	is the final infiltration capacity (LT^{-1}) ,
3128	f_d	decay factor (L ⁻¹)
3129	f_0	initial infiltration capacity (LT ⁻¹)
3130	f _{h20sfc}	fraction of the area that is inundated (-)
3131	f_H	Hortonian infiltration capacity at time t (LT^{-1})
3132	f_m	maximum potential infiltration rate (LT ⁻¹)
3133	f_{mm}	average potential infiltration rate (LT ⁻¹)
3134	f _{sno}	fraction of the grid cell covered by snow (-)
3135	$f_{{ m sc},i}$	fraction of soil carbon in layer <i>i</i> ,
3136	f _{unf,i}	pdf representing the spatial variability of the local maximum infiltration rate in a grid cell
3137	$f_s(s)$	gamma function of the mean surface layer point soil water saturation
3138	h _{sat}	pressure head at air entry value (L)
3139	I _{max}	maximum infiltration rate (ML ² T ⁻¹ or LT ⁻¹) or maximum soil moisture capacity (L)
3140	I _{c,t}	cumulative infiltration capacity at a certain moment in time t (L)
3141	I _{unf,i}	local maximum infiltration rates for unfrozen soil at soil layer I (LT ⁻¹)
3142	i	point soil moisture capacity (L)
3143	i _c	infiltration capacity (ML ² T ⁻¹)
3144	Ι	spatially averaged actual infiltration (LT ⁻¹)
3145	$\langle I_m \rangle$	mean maximum infiltration rate over the grid cell
3146	I roff	normalized runoff in SSiB (LT ⁻¹)
3147	h	matric potential (L)
3148	h_A	minimum (i.e., for evaporation) pressure head at the soil surface allowed under the prevailing
3149		soil conditions [L]
3150	hs	maximum (i.e., for infiltration) pressure heads at the soil surface allowed under the prevailing
3151	,	soil conditions [L]
3152	h_c	matric potential at air entry (L)
3153	n_f	capillary pressure at the wetting front [L],
3154	$h_o(t)$	matric potential at the soil surface at time t (I)
3155	н	total water head (L)
3156	ι_p	maximum potential rate of infiltration or evaporation under the current atmospheric conditions
3157		
3158	 ;*(+)	point scale water capacity (L)
3159	l (l) I*	scaled infiltration rate (L1 ⁻)
2161	I	infiltration rate for the whole coil column (LT^{-1})
2162	I_{γ}	local maximum infiltration rates for unfregen soil (LT ⁻¹)
2162	¹ unf,i	Dereign water flux $(1 T^{-1})$
2167	J	Darcial water flux (LT) procinitation rate $[I, T^{-1}]$
2165	J _w ⊮int	precipitation rate [L T] average of hydraulic conductivity at the wetting front and the deepest saturated node (IT^{-1})
2102	Γ _i wint.*	average of hydraulic conductivity at the wetting from and the deepest saturated hode (Γ)
3166	K_i	scaled $K_i^{(i)}(LT)$
310/	Λ _{dt} ν	constant parameter set equal to 3.0 (-) reference $K_{\rm M2}$ (2×10^{-6} m/s) (1.7 ⁻¹)
31C0	п _{ref} V	$\frac{1}{1}$
3109	Λ _S V	saturated hydraulic conductivity (L1 ⁻)
31/U 2171	Λ _{s,min,i} ν	saturated hydraulic conductivity of the organic cell certain of layer I (LI ⁻)
31/1	п _{s,sc,i}	saturated hydraulic conductivity of the organic soll carbon of layer I (LT *)

3172	Ko	hydraulic conductivity of the soil surface layer (LT ⁻¹)
3173	1	tortuosity index in the Mualem model (-)
3174	Mse	surface layer excess [L]
3175	т	fitting parameter in the van Genuchten model (-)
3176	n_{vg}	pore size distribution index in van Genuchten model (-)
3177	n_{K}	fitting parameter in the Kostiakov Equation
3178	P _{drop}	precipitation reaching surface after canopy interceptrion in SSiB (LT ⁻¹)
3179	P_M	snowmelt (either L or ML ² T ⁻¹ or LT ⁻¹)
3180	P_R	rainfall rate (LT ⁻¹)
3181	P_T	throughfall precipitation (either L or ML ² T ⁻¹ or LT ⁻¹)
3182	P_{x}	flux incident at the soil surface (ML ² T ⁻¹),
3183	q_{cav}	infiltration capacity of the soil (LT ⁻¹)
3184	q(t)	infiltration flux (LT ⁻¹)
3185	$q^*(t)$	scaled infiltration rate (LT ⁻¹)
3186	q_f	final (constant) infiltration rate (L T ⁻¹)
3187	q_i	initial infiltration rate (L T ⁻¹)
3188	q _{evapo} .	soil water loss due to evaporation (LT ⁻¹)
3189	q _{in soil}	infiltration rate of water into the soil (LT ⁻¹)
3190	q_s	surface runoff (ML ² T ⁻¹) or (LT ⁻¹)
3191	q_H	Hortonian excess infiltration runoff (LT ⁻¹)
3192	q_D	Dunne saturation excess runoff (LT ⁻¹)
3193	$q_{lia.o}$	moisture input into the grid cell (LT ⁻¹) and is the sum of liquid precipitation reaching the surface
3194	17	and snowmelt
3195	$q_{in.sur}$	_{face} surface moisture flux remaining after surface runoff has been removed (LT ⁻¹)
3196	q_{1}	downslope subsurface flow rate per unit contour width (LT ⁻¹)
3197	q_{re}	recharge rate (LT ⁻¹)
3198	Q(t)	cumulative infiltration at time t [L]
3199	Q_{wat}	input of water (rainfall, snowfall, dew) (LT ⁻¹)
3200	r(t)	water supply rate (LT ⁻¹)
3201	r_o	amount of water that needs to infiltrate (throughfall, snowmelt and ponded water) (LT ⁻¹)
3202	R(i)	mean infiltration excess runoff (LT ⁻¹)
3203	5	water content expressed as saturation (-)
3204	$\langle s \rangle$	grid mean surface layer soil water saturation (-)
3205	S	grid cell mean storage (-)
3206	S_e	the effective saturation (-)
3207	S_g	surface gradient (-)
3208	S_{max}	maximum water depth over the basin (L)
3209	So	minimum storage below which there is no surface saturation (L)
3210	S_{op}	soil sorptivity [L T ⁻²],
3211	SW	equilibrium root zone wetness index (-)
3212	SWo	minimum value of the soil wetness index distribution (-)
3213	SWI	Soil water index (-)
3214	SI	mean slope in the grid-cells
3215	SI _{max}	maximum threshold slope
3216	$S_{x_l}^*$	local terrain surface slope
3217	t	time (T)
3218	Т	transmissivity (LT ⁻¹)

3219	T_o	transmissivity of the soil profile (LT ⁻¹)
3220	t^*	scaled time (T)
3221	t_f	time needed to infiltrate a certain amount of water (T)
3222	t_p	time to ponding (T)
3223	$T(z_{\nabla})$	transmissivity in Eq. [A38]
3224	tanβ	local surface topographic slope
3225	\vec{v}	depth averaged velocity vector [LT ⁻¹],
3226	v_{κ}	parameter describing the decrease of saturated hydraulic conductivity with depth
3227	Wmin	minimal local subgrid soil water capacity
3228	Wmax	maximum local soil water capacity
3229	Wact	subgrid water content that corresponds to the fractional saturation
3230	W	vertically integrated soil water content (θ) over the first 50 cm of the soil profile (L)
3231	W_{sat}	vertically integrated saturated soil water content (θ_{sat}) over the first 50 cm of the soil profile (L)
3232	\bar{x}	mean catchment value of $ln(\alpha/tan\beta)$
3233	Х	dimensionless time
3234	z(i)	thickness of soil layer <i>i</i> (L)
3235	Z _{ndm}	depth over which soil moisture is considered (L)
3236	Z	soil profile depth to bedrock (L)
3237	Z_{a}	ground surface elevation (L)
3238	Zm	maximum value of profile depth to bedrock (L)
3239	Z_{∇}	mean water table depth (L)
3240	Z_1	local water table depth (L)
3241	Zhot	middle point of the bottom layer (1.5.m) (L)
3242	Z _{wt}	water table depth (L)
3243	α_{an}	anisotropic factor accounting for differences in Ksat between vertical and horizontal direction
3244	α_G	parameter in the Gamma distribution
3245	α_{GA}	, parameter proportional to the matric potential at the wetting front
3246	β_G	parameter in the Gamma distribution
3247	α_{AC}	Miller-Miller scaling factor for final infiltration capacity
3248	α_{K}	decay constant in Kostiakov equation
3249	α_s	shape parameter in the spatial distribution function of soil wetness
3250	α_{sc}	Miller-Miller similarity scaling factor
3251	α_{Son}	Miller-Miller scaling factor for sorptivity
3252	α_{ont}	single Miller-Miller scaling factor for infiltration
3253	α_T	upstream area that contributes flow through a unit contour positioned at the point or specific
3254	1	catchment area
3255	α_{wf}	product of the absolute value of wetting front suction head and the difference between
3256	WJ	saturated water content and initial water content at the beginning of the infiltration event
3257	β_{T}	slope parameter
3258	B	parameter depending on grid resolution (-)
3259	r Br	fitting parameter in the Kostiakov equation
3260	B	correction parameter for Ks (-)
3261	rs V	parameter related to topography (-)
3262	r Vf	fraction of surface runoff (-)
3263	$\gamma_{1,2,2}$	fitting parameters
3264	r1,2,3 δ.	model time sten (L)
3265	s S	dimensionless error (-)
5205	c	

3266	θ	volumetric soil water content (-)
3267	θ_l	the content of liquid water (-)
3268	θ_{ice}	the content of ice (-)
3269	θ_i	initial water content (-)
3270	θ_s	saturated soil water content (-)
3271	$ heta_r$	residual moisture content (-)
3272	θ_{rz}	mean diagnosed root zone moisture content [-]
3273	θ_{wilt}	water content at wilting point (-)
3274	κ_p	related to the standard deviation of the subgrid slope (-)
3275	κ	scaling factor needed to redistribute the GCM grid scale precipitation over the scale of
3276		precipitation events (-)
3277	λ	wetness index (-)
3278	λ_{sc}	characteristic length of a Miller-Miller similar porous medium (L)
3279	λ_{crit}	critical topographic index (-)
3280	λ_p	dimensionless pore size distribution index [-]
3281	λ_m	mean topographic or wetness index (-)
3282	λ_s	subgrid heterogeneity of soil (-)
3283	λ_r	characteristic length of Miller-Miller scaling reference soil (L)
3284	ρ	correlation coefficient between the terrain slope and the soil water content (-)
3285	σ_{or}	standard deviation of the orography
3286	σ_{min}	minimum standard deviation of the orography
3287	σ_{max}	maximum standard deviation of the orography
3288	σ_{slope}	standard deviation of the subgrid slope variability (-)
3289	$\sigma_{ heta}$	standard deviation of soil water content (-)
3290	$\sigma_{S_{x_1}}$	standard deviation of local surface slopes (-)
3291	σ_{Ks}	standard deviation of saturated hydraulic conductivity (LT ⁻¹)
3292	τ	time scale of transfer of surface layer moisture into the root zone (T)
3293	а	fraction of surface runoff
3294		

3295 Appendix

3296

3298

3297 Appendix A1: The PDM of Moore (1985)

3299 In the PDM-based scheme (Moore, 1985) for calculating Dunne runoff, *F*_{sat} was described as:

3300
$$F_{sat} = 1 - \left(1 - \frac{\langle S \rangle - S_0}{S_{max} - S_0}\right)^{b/(b+1)}$$
 [A1]

where $\langle S \rangle$ is the grid cell mean water storage [L], S_0 is the minimum water storage below which there is no water saturation at the surface [L], S_{max} is the maximum possible grid cell water storage [L], and *b* is a shape parameter proposed by Moore (1985) that reflects the heterogeinity in a lumped manner (see also Eq. 64). Parameters *b* and S_o were obtained from model calibration using catchment data and S_{max} was obtained from available data and calculated from:

$$3306 \qquad S_{max} = \theta_{sat} z_{pdm}$$
[A2]

3307 where z_{pdm} (L) is the soil depth over which the soil water content is considered for PDM modelling. Clark 3308 and Gedney (2008) assumed z_{pdm} to be 1 m.

3309 Appendix A2: Description of maximum infiltration rate in different LSMs

Note that only those models using the maximum infiltration rate in their concept will be described here and that the last number of the label (e.g., A2.**3**) referes to the number given in Table 1 to facilitate reading. Additionally, I_{max} depends on F_{sat} for those models relying on the F_{sat} approach.

3313 A2.3 ORCHIDEE

ORCHIDEE (Ducharne et al., 2017) includes a sub-grid distribution of infiltration, which reduces the effective infiltration rate into each successive layer of the wetting front. In practice, the mean infiltrability of a layer over the grid-cell is spatially distributed using an exponential pdf, then compared locally to the amount of water that needs to infiltrate (called r_o and comprised of throughfall, potentially increased by snowmelt and ponded water). As a result, infiltration-excess runoff is produced over the fraction of the grid-cell where r_o [L T⁻¹] is larger than the local K_i^{int} [L T⁻¹] defined by the exponential distribution of mean saturated hydraulic conductivity $\langle K_i^{int} \rangle$, applying the following cumulative distribution function (cdf):

3321
$$F(K_i^{int}) = 1 - exp^{\left(-\frac{K_i^{int}}{\langle K_i^{int} \rangle}\right)}$$
[A3]

3322 K_i^{int} is calculated as the average of the actual hydraulic conductivity at the wetting front and the deepest 3323 saturated node. A spatial integration is conducted for each soil layer that becomes saturated when the 3324 wetting front propagates, giving the mean infiltration excess runoff *Re*, *i* produced from the saturation of 3325 each soil layer *i*:

3326
$$R_{e,i} = r_o - K_i^{int} (1 - \exp^{(-\frac{r_o}{K_i^{int}})})$$
 [A4]

By reducing the effective conductivity $K_i^{int,*} = K_i^{int}(1 - exp^{(-\frac{r_o}{K_i^{int}})})$ compared to the uniform case ($K_i^{int,*} = K_i^{int}$), this sub-grid distribution increases surface runoff, given by the sum of R_i from all the layers saturated during the time step. The model also considers the mean slope of the grid-cell, with a reinfiltration of excess water only possible at low slopes. This sub-grid distribution can be seen as the opposite to the parametrization of Warrilow et al. (1986), since the actual hydraulic conductivity K rather than the precipitation rate is spatially distributed within the grid-cells.

3333 A2.4 CLSM

3334 The Catchment Land Surface Model (CLSM) (Koster et al., 2000), the land model component of the NASA 3335 Goddard Earth Observing System (GEOS-5) coupled Earth system model, does not impose a priori a 3336 maximum infiltration rate in its formulation. The amount of water that can infiltrate over a certain time 3337 at the catchment scale is a function of the model's dynamically varying spatial moisture fields. Infiltration 3338 in CLSM is considered here in two steps: (i) precipitation throughfall into the near-surface soil layer (2 or 3339 5 cm), and (ii) the subsequent transfer of this soil water into the root zone. It is important to recognize 3340 that CLSM is designed to emphasize a description of horizontal moisture variability that is linked to the 3341 simulation of a spatially-variable dynamic water table depth. This is discussed in more detail in Section 3342 4.1.2. In effect, the land surface area in CLSM is divided into distinct (and dynamically changing) 3343 hydrological regimes. Regarding the throughfall into the near-surface layer, all rainwater runs off the 3344 surface in the 'saturated fraction' regime, effectively as Dunne runoff and without infiltration. In recent 3345 versions of CLSM, the other two regimes (the 'subsaturated-but-transpiring' and the 'wilting' regimes) 3346 allow all precipitation water in a given time step to infiltrate, and thereby, increase the surface soil 3347 moisture, though if the layer becomes fully saturated, the excess does run off the surface, effectively as 3348 Hortonian runoff.

The transfer of surface layer moisture into the root zone is controlled by a time scale, τ [T], computed with
3350 $\tau = a_r / (\theta_{rz} + b_r M_{se})^3$.

[A5]

here, a_r and b_r are fitted parameters, θ_{rz} is mean diagnosed root zone moisture content [L³ L⁻³] and M_{se} is the surface layer excess [L] (see Section 4.1.2). With this timescale defined, the water transferred from the surface layer to the root zone, ΔM_{se} [L], is

$$3354 \quad \Delta M_{se} = -M_{se} \Delta t / \tau$$
 [A6]

The empirical equation for the timescale τ was fitted to results from high resolution (1 cm) solutions of the vertical one-dimensional Richards equation, conducted off-line prior running climate or land surface simulations. The simulations behind these offline solutions used a comprehensive set of values for the CLSM's water prognostic variables (see Ducharne et al., 2000) appropriately downscaled to 1 cm vertical resolution, and a comprehensive set of soil classes parameterized by the Campbell (1974) equations, with corresponding hydraulic parameters based on lookup tables or using the pedotransfer functions (PTFs) of Wösten et al. (2001) (de Lannoy et al., 2014).

3362 In CLSM, catchment-scale infiltration rate decreases by two mechanisms in which the actual groundwater 3363 level is crucial: 1) the non-saturated area into which rainfall can infiltrate at the catchment scale decreases 3364 for rising water levels, i.e. higher areal fractions of the saturated regime, and 2) the hydraulic gradient 3365 between surface and root zone in the non-saturated area decreases when the root zone fills up due to 3366 infiltration and rising water levels. The combination of both mechanisms results in a dynamical prediction 3367 of catchment scale maximum infiltration rates into the surface layer that range from high values (larger 3368 than K_s) under deep water level conditions to values that drop below K_s under shallow water level 3369 conditions.

3370 A2.5 ISBA-SURFEX

In ISBA-SURFEX (Decharme and Douville, 2006), the local maximum infiltration rates for unfrozen soil aregiven by:

3373
$$I_{unf,i} = K_{s,i} \left[\frac{b_{BC}h_c}{\Delta z} \left(\frac{\theta}{\theta_s} - 1 \right) + 1 \right]$$
[A7]

where h_c is the matric potential at air entry [L], θ_s is the soil porosity or saturated water content [L³ L⁻³], b_{BC} is the pore size distribution index from the the Brooks Corey equation [-] (see Eq. [4]), Δz is the top layer soil thickness of 0.1m, and $K_{s,i}$ is the saturated hydraulic conductivity at location *i* [L T⁻¹]. $I_{unf,i}$ comes from the equation presented in the paper by Abramopoulos et al. (1988) for calculating infiltration
and evapotranspiraton in global climate models, whereby the maximum infiltration was defined as:

3379
$$I_{max} = K_{s,i} \left[\frac{dh_i}{d\theta_i} \Big|_{\theta_i = \theta_s} \left(\frac{\theta_i - \theta_s}{z_i} \right) + 1 \right]$$
 [A8]

where *i* refers to the top soil layer (*i* = 1), θ_i the volumetric soil water content of top soil layer [L³ L⁻³], and z_i the thickness of this layer [L]. The mean maximum infiltration rate, $\langle I_{max} \rangle$ is used to calculate the surface runoff generated by Hortonian overland flow as:

3383
$$q_{H} = \mu \left[\int_{0}^{1} \int_{f^{*}}^{\infty} (P_{x,i} - I_{unf,i}) f_{Px,i}(P_{x,i}) dP_{x,i} f_{unf,i}(I_{unf,i}) dI_{unf,i} \right]$$
[A9]

3384 where P_{χ} is the incident flux reaching the the soil surface and

3385
$$f_{unf,i}(I_{unf,i}) = \frac{1}{\langle I \rangle} e^{-I_{max,i}/\langle I_{max} \rangle}$$
[A10]

3386 where $\langle I_{max} \rangle$ is the mean maximum infiltration rate over the grid cell [L T⁻¹]. Hereby, $f_{unf,i}(I_{unf,i})$ 3387 represents the spatial variability of the local maximum infiltration rate in a grid cell.

3388 The parameter μ in Eq. [58] is given by:

$$\mu = 1 - e^{-\beta \langle P_X \rangle}$$
[A11]

3390 where β is a parameter depending on the grid resolution according to:

3391
$$\beta = 0.2 + 0.5e^{-0.01dx}$$
 [A12]

- 3392 where *dx* is the length of the grid cell in km.
- 3393 Combining all equations, we obtain:

3394
$$q_H = \frac{\langle P_X \rangle}{1 + \langle I_{unf} \rangle \frac{\mu}{\langle P_X \rangle}}$$
[A13]

Overall, the infiltration rate is calculated from the difference between throughfall rate and surface runoff,
whereby the throughfall rate has three components, namely interception, snowmelt, and dripping from
the interception reservoir.

3398 A2.6 Noah-MP

3399 Wang et al. (2016) defined the maximum infiltration rate, *I*_{max} [L T⁻¹], for a grid cell in Noah-MP as:

3400
$$I_{max} = \frac{P_x D_x [1 - \exp(-kdt\delta_t)]}{P_x + [1 - \exp(-kdt\delta_t)]}$$
 [A14]

3401 where δ_t is the model time step [T]. D_x is incorrectly termed by Wang et al. (2016) as soil water diffusivity, 3402 when in fact it is simply the soil water storage in length units (L), calculated as:

3403
$$D_x = \sum_{i=1}^4 \Delta z_i (\theta_s - \theta_i)$$
[A15]

3404 and

$$3405 kdt = kdt_{ref} \frac{K_s}{K_{ref}} aga{A16}$$

where P_{χ} is defined as the precipitation rate [L T⁻¹], K_s is the saturated hydraulic conductivity [L T⁻¹], θ_s and θ_i are the volumetric saturated water content and the actual water content [L³ L⁻³] at time step *i*, respectively. *Kdt* is a parameter in Eq. [A14], K_{dtref} is constant parameter set equal to 3.0 (-), and K_{ref} is a reference *K* value (2x10⁻⁶ m s⁻¹).

3410 In Noah-MP (Niu et al., 2005, Niu et al., 2011b) I_{max} is used to calculate Hortonian excess infiltration using 3411 the following equation:

3412
$$q_s = F_{sat}Q_{wat} + (1 - F_{sat})\max(0, (Q_{wat} - I_{max}))$$
 [A17]

where F_{sat} is calculated from the TOPMODEL (see below), Q_{wat} [L T⁻¹] is the input of water (rainfall, snowfall, dew) and I_{max} is the maximum soil infiltration capacity calculated according to Entekhabi and Eagleson (1989), where it is defined as infiltrability.

3416 A2.7 JULES

3417 In the JULES model (Best et al., 2011) the maximum surface infiltration rate is defined as $I_{max} = \beta s K_s$, where 3418 βs is the enhancement factor [-], generally set equal to 0.5 for bare soil, whereas larger values are used 3419 for vegetated grid cells (4 for trees, 2 for grasses and shubs), to account for infiltration enhancing factors 3420 such as root macropores, and K_s is the saturated hydraulic conductivity [L T⁻¹]. This approach may lead to 3421 an underestimation of the infiltration rate as sorptivity forces are not taken into account and essentially 3422 all the water reaching the soil surface will infiltrate. Hortonian runoff is calculated as the difference 3423 between throughfall plus snowmelt and infiltration. Runoff can increase under certain configurations to 3424 avoid supersaturation of the upper soil layer - thus explicitly representing Dunne runoff at the point scale. 3425 If the 'large scale hydrology' scheme is used, Dunne runoff is calculated in addition to Hortonian runoff, 3426 based on the surface saturated fraction, F_{sat} (see Appendix A3), according to:

 $3427 \qquad q_{\text{dunne}} = F_{sat} q(t)$

[A18]

3428 where q(t) is the infiltration rate [L T⁻¹], which is multiplied by 1 - F_{sat} to account for this additional runoff 3429 term. Note, that ponding is not simulated.

3430 A2.8 CLM

The Community Land Model (CLM) 4.5 version (Oleson et al., 2013) calculates the maximum soil infiltration capacity as:

3433
$$I_{max} = (1 - F_{sat})K_sC_{ice}$$
 [A19]

3434 where K_s is the saturated hydraulic conductivity [L T⁻¹], and C_{ice} is an ice impedance factor [-]. Hortonian 3435 excess infiltration runoff, q_H [L T⁻¹], is generated as:

3436
$$q_H = \max(q_{in,soil} - (1 - f_{h20sfc})I_{max}, 0)$$
 [A20]

where f_{h20sfc} is the fraction of the area where ponded water exists exists and thus equals F_{sat} . Note, that Hortonian excess infiltration runoff is only generated and ponded water only occurs on the diagnosed unsaturated fraction (1-Fsat) of the soil column. $q_{in,soil}$ refers to the infiltration rate of water into the soil, defined as:

3441
$$q_{in,soil} = (1 - f_{h20sfc})q_{in,surface} - q_H - (1 - f_{sno} - f_{h20sfc})q_{evapo,soil}$$
 [A21]

3442 and

3443
$$q_{in,surface} = (1 - F_{sat})q_{liq,o}$$
 [A22]

where $q_{liq,o}$ is the water input into the grid cell [L T⁻¹] that is the sum of liquid precipitation reaching the surface and snowmelt. $q_{evapo,soil}$ [L T⁻¹] is the water loss due to evaporation, $q_{in,surface}$ [L T⁻¹] is the surface water flux after surface runoff has been removed, and f_{sno} is the fraction of the grid cell covered by snow.

3448 A2.11 H-TESSEL/CH-TESSEL

In H-TESSEL (Balsamo et al., 2009) or in the more recent CH-TESSEL both based on the same hydrological
principles (Boussetta et al., 2013) the maximum infiltration rate is calculated using Eq. [A23] to calculate
Hortonian overland flow.

3452
$$I_{max} = (W_{sat} - W) + max \left(0, W_{sat} \left\{ \left(1 - \frac{W}{W_{sat}} \right)^{\frac{1}{b+1}} - \left(\frac{P_T + P_M}{(b+1)W_{sat}} \right)^{\frac{1}{b+1}} \right)$$
[A23]

where P_T is the throughfall precipitation [L], P_M is the snowmelt [L] leading to P_x as the total water reaching the surface ($P_x = P_T + P_M$) [L], and W and W_{sat} [L] are the vertically integrated soil water contents (equivalent to θ and θ_s , albeit with different units) over the first 50 cm of the soil profile. The *b* parameter reflects the grid cell heterogeneity (see Section 4.1.2). In H-TESSEL/CH-TESSEL $q_s = P_x - I_{max}$, where q_s is surface runoff (defined as *R* in Balsamo et al. (2009)). Notice that the units of I_{max} are length, although it is defined as a rate in Balsamo et al. (2009).

3459 A3 Description of the saturated water fraction *F*_{sat}

Note that only those models using the maximum infiltration rate in their concept will be described here and that the last number of the label (e.g., A3.3) referes to the number given in Table 1 to facilitate reading. As the TOPMODEL concept to calculate F_{sat} is embedded in several LSMs presented in this appendix, we briefly present the basic equations and ways to calculate basic properties.

3464 A3.0 TOPMODEL

3465 In the TOPMODEL approach (Niu et al., 2005) F_{sat} can be defined as:

3466
$$F_{sat} = \int_{\lambda \ge (\lambda_m + f_d z_{\nabla})} p df(\lambda) d\lambda$$
 [A24]

where f_d is the decay factor (L⁻¹), which is a measure for the decline of K_s with increasing depth, z_{∇} is the mean water table depth, and the local water table depth z_l is given by:

3469
$$z_l = z_{\nabla} - \frac{1}{f_d} (\lambda_m - \lambda)$$
 [A25]

3470 Here, the mean topographic or wetness index λ_m is defined as:

3471
$$\lambda_m = \langle ln(\alpha_T/tan\beta_T) \rangle$$
 [A26]

3472 where α_T is the specific catchment area and $tan\beta_T$ is the local surface topographic slope.

3473 In order to calculate the average water table depth Chen and Kumar (2001) proposed an iterative 3474 procedure where D_{θ} is the amount of water stored between surface and groundwater:

3475
$$D_{\theta} = \int_{0}^{z_{\nabla}} (\langle \theta_{s}(z) \rangle - \langle \theta(z) \rangle) dz$$
 [A27]

3476 where the water contents $\theta_s(Z)$ and $\theta(Z)$ denote the catchment or basin average [L³ L⁻³]. Further, D_{θ} is 3477 calculated from:

3478
$$D_{\theta} = \sum_{i=1}^{NLAYERS} (\theta_s - \langle \theta(z) \rangle_i) \Delta z_i$$
 [A28]

The water content $\theta(z)$ is calculated using e.g. the Brooks Corey equation (Eq. [4-6]) and the assumption that the soil water content profile is an equilibrium with the groundwater by:

3481
$$\langle \theta(z) \rangle = \theta_s \left(\frac{h_c - (z_{\nabla} - z)}{h_c}\right)^{-1/B'}$$
 [A29]

3482
$$\langle \theta(z) \rangle = \langle \theta_s(z) \rangle \left(\frac{h_c - (z_{\nabla} - z)}{h_c} \right)^{-1/B'}$$
 [A30]

3483 where *B*' is related to the Brooks Corey exponent of the water retention characteristic and h_c is the 3484 pressure head at air entry [cm]. This approach was used by Niu et al. (2005) to develop a runoff-scheme 3485 for global climate models and it has also been implemented in CLM (see A3.8)

3486 **A3.3 ORCHIDEE**

The ORCHIDEE model does not use F_{sat} to generate surface runoff, which is the complement of upscaled local infiltration rates (see A2.3). In constrast, it uses the concept of ponded fraction, to reduce surface and enhance infiltration. A fraction of surface runoff, γ_f , is allowed to pond in flat areas, and it is kept to be infiltrated at the following time step with throughfall and snowmelt, to account for the effect of ponding on infiltration (d'Orgeval et al., 2008). This fraction γ is constant over time, but varies spatially, based on the mean slope *SI* in the grid-cells and a threshold slope SI_{max} (with a default value of 0.5%), such that the ponding fraction decreases from 1 when SI = 0 to 0 when $SI \ge SI_{max}$:

3494
$$\gamma_f = 1 - \min(1, Sl/Sl_{max}).$$
 [A31]

This leads to reduce grid-scale surface runoff by γ_f .

3496 A3.4 Catchment Land Surface Model (CLSM)

In the Catchment Land Surface Model, the saturated land fraction at equilibrium conditions is effectively
computed as the fraction of the area for which the water table depth lies "above" the ground surface,
based on the TOPMODEL framework. The strategy for calculating the saturated land fraction was
described above in Section 4.1.2.

3501 A3.5 ISBA-SURFEX

3502 In the ISBA-SURFEX model, the saturation excess runoff can also be computed using the TOPMODEL 3503 assumption instead of using the Arno scheme. So, only Dunne runoff is affected by F_{sat} (Decharme and Douville, 2006) and it is described according to a corrected approach of the original TOPMODEL framework proposed by Saulnier and Datin (2004) and written as:

$$3506 \quad q_D = P_x F_{sat} \tag{A32}$$

where F_{sat} is defined as the saturation fraction of a grid cell, being inversely proportional to the mean water storage deficit, D_t , of the grid cell, whereby D_t can be written as:

3509
$$D_t = (\theta_s - \langle \theta \rangle) \langle d_2 \rangle$$
 [A33]

3510 D_t is bounded between 0 and d_o , the maximum local water deficit defined by:

$$3511 \quad d_{\rho} = (\theta_{s} - \theta_{wilt}) \langle d_{2} \rangle$$
 [A34]

where θ_s and $\langle \theta \rangle$ are the saturated and mean volumetric water content averaged over the depth d_2 [L] at grid scale [L³ L⁻³] that can be, optionally, the depth of the entire root zone (Decharme and Douville, 2006) or the depth of the layer in which the cumulated root profile reached 90% (Decharme et al., 2013) and θ_{wilt} is the water content at wilting point [L³ L⁻³]. Hereby, D_t will be d_o when $F_{sat} = 0$ or vice versa

3516 A3.6 Noah, Noah-MP

3517 In this section we briefly describe the way infiltration is handled in NOAH and then present Noah-MP and 3518 the approaches used to calculate F_{sat} .

In the NOAH model (Schaake et al., 1996), the spatially averaged actual infiltration rate, *Ir*, depends on the cumulative infiltration capacity ($I_{c,t}$) at a certain moment in time *t*. $I_{c,t}$ is expressed as:

3521
$$I_{c,t} = D_b [1 - \exp(-K_{dt}\Delta t)]$$
 [A35]

3522 where Δt is the model time step, K_{dt} is a constant, and D_b represents the spatially averaged soil water 3523 storage for the whole soil column. D_b in each soil layer is computed by:

3524
$$D_b(i) = D_{bmax}(i)\left(1 - \frac{\theta_l(i) + \theta_i(i) - \theta_{wilt}(i)}{\theta_s(i) - \theta_{wilt}(i)}\right)$$
[A36]

where $D_{bmax}(i)$, $\theta_l(i)$, $\theta_i(i)$, $\theta_{wilt}(i)$ and $\theta_s(i)$ are the maximum soil water storage, the content of liquid water and ice, wilting point, and soil porocity or saturated water content in soil layer *i*, respectively. $D_{bmax}(i)$ is defined by the following equation:

3528
$$D_{bmax}(i) = -z(i)(\theta_s(i) - \theta_{wilt}(i))$$
[A37]

3529 where z(*i*) is the thinkness of soil layer *i*.

3530 Then, the infiltration rate for the whole soil column is given by:

3531
$$I_r = (\frac{P_R * I_{c,t}}{P_R + I_{c,t}}) / \Delta t$$
 [A38]

3532 where *PX* is the precipitation input into the whole column.

Soil freezing has significant effect on the permeability of soils because ice impedes the infiltration rate.
Noah computs the impermeable area factor *FC* to consider freezing influence on soil infiltration following
Koren et al. (1999).

- Soil freezing has significant effect on the permeability of soils because ice impedes the infiltration rate.
 Noah computs the impermeable area factor *FC* to consider freezing influence on soil infiltration following
 Koren et al. (1999).
- Noah-MP is an improved version of Noah (Niu et al., 2011b), whereby Noah-MP (Niu et al., 2011b) offers four options for computing infiltration and surface-subsurface runoff. Option 1 is the TOPMODEL-based runoff scheme with the simple groundwater scheme (Niu and Yang, 2007) implemented by Cai et al. (2014), where the fraction of the gridbox that is saturated, F_{sat} , is given by:

3543
$$F_{sat} = (1 - F_{frz})F_{max}e^{-0.5f_d(z_{wt} - z_{bot})} + F_{frz}$$
[A39]

where z_{bot} is the soil profile thickness (default = 2.0 m), z_{wt} (L) is the water table depth, F_{max} is set to a global mean value of 0.38, and F_{frz} is the fraction of impermeable area as a function of soil ice content of the surface soil layer. At urban areas F_{frz} is set to 0.95. The runoff decay factor, f_d , in Eq. [A39] equals 6 m⁻ 1.

Option 2 is a simple TOPMODEL-based runoff scheme with an equilibrium water table (Niu et al., 2005). Like in Option 1, this scheme parameterizes both surface and subsurface runoff as functions of the water table depth but with a sealed bottom of the soil column (zero-flux lower boundary condition) in accordance with one of the TOPMODEL assumptions, i.e., the exponential decay of saturated hydraulic conductivity, F_{sat} is calculated as:

3553
$$F_{sat} = (1 - F_{frz})F_{max}e^{-0.5f_d z_{wt}} + F_{frz}$$
 [A40]

3554 here, f_d is set to 2.0 m⁻¹.

Option 3 is an infiltration-excess-based surface runoff scheme with a gravitational free-drainage subsurface runoff scheme as used in the original Noah (Schaake et al., 1996). Surface runoff (*R*) is computed as the excess of precipitation (P_d) not infiltrated into the soil ($R = P_d - I_{max}$). The maximum infiltration rate, I_{max} , is computed as:

3559
$$I_{max} = P_d \frac{D_x(1 - e^{-kdt\Delta t})}{P_d + D_x(1 - e^{-kdt\Delta t})}$$
 [A41]

3560 with

$$3561 D_x = \sum_{i=1}^N \Delta z_i (\theta_s - \theta_i) [A42]$$

3562 and

$$3563 \quad kdt = kdt_{ref} \frac{K_S}{K_{ref}}$$
[A43]

where Δt is the time step (T), and K_s (L T⁻¹) is the saturated hydraulic conductivity, which depends on soil texture and is prescribed in a lookup table. The symbol *N* stands for the number of layers. The parameters $kdt_{ref} = 3.0$ and $K_{ref} = 2 \times 10^{-6}$ m s⁻¹ were determined in the framework of the PILPS2(c) experiments for the Red-Arkansas River basins in the Southern Great Plains region of the United States (Wood et al., 1998). Finally, option 4 is the BATS runoff scheme, which parameterizes surface runoff as a 4th power function of the top 2 m soil wetness (expressed as degree of saturation) and subsurface runoff as gravitational free drainage (Yang and Dickinson, 1996) described by:

3571
$$F_{sat} = \left(1 - F_{frz}\right) \left(\frac{\theta_{tot}}{\theta_s}\right)^4 + F_{frz}$$
[A44]

3572 with

3573
$$\theta_{tot} = \frac{1}{z_{bot}} \sum_{i=1}^{N} \Delta z_i \theta_i$$
 [A45]

3574 A3.7 JULES

There are two options in JULES to account for spatial heterogeneity of soil water content and thus determine F_{sat} . The first option is based on a modified form of the TOPMODEL (Beven and Kirkby, 1979), described by Gedney and Cox (2003), where the assumption of an exponential decay of K_s with depth (leading to Eqs [A24-A25]) is relaxed. Gridbox mean water table depth, z_{∇} , is calculated using the approach described in A3.0 (Eqs [A27-A29]). This is used to estimate a critical topographic index λ_{crit} using the relation:

$$\lambda_{crit} = \ln(T(0) / T(z_{\overline{V}})) + \lambda_m$$
[A46]

3582 where transmissivity $T(z_{\nabla})$ is given by:

$$3583 T(z_{\nabla}) = \int_{z}^{\infty} K_{s}(z) dz [A47]$$

3584 F_{sat} is then calculated as the fraction of the gridbox for which $\lambda > \lambda_{crit}$, assuming λ follows a gamma 3585 distribution with mean (λ_m) and standard deviation read in from observational datasets. In order to speed 3586 up the computation, the integral over the probability distribution of λ is calculated for a range of mean 3587 water table depths during model initialisation, and approximated by an exponential function by:

$$F_{sat} = a_s exp\left(-c_s \lambda_{crit}\right)$$
[A48]

where a_s and c_s are fitted to approximate the full integral (i.e. Eq. [A24]). Recently, this scheme has been modified to account for the impact of frozen water in the soil by replacing K_s in Eq. [A49] by $(1-\theta_f)^{2b+3}K_s$ (where *b* is the Brooks-Corey parameter ,and θ_f is the frozen water content) and additionally correcting the gridbox mean water table depth (z_{∇}) to account for the fact that the profile of soil moisture above the water table will not follow the same equilibrium profile (assumed in Eq. [A29]) when ice is present. The second option for calculating F_{sat} is the use of the probability distributed model of Moore (1985) (see Eq. [38]).

3596 A3.8 CLM 4.5

In CLM 4.5 (Lawrence et al., 2011, Oleson et al., 2013), the fraction of the saturated area, *F_{sat}* is calculated
 by:

3599
$$F_{sat} = F_{max} exp(-0.5 f_d z_{\nabla})$$
 [A49]

where F_{max} is the maximum value of F_{sat} and f_d is the decay factor (L⁻¹) F_{max} is defined as the fraction of sub-grid cells from a high-resolution digital elevation map (DEM) in a grid cell whose topographic index (the ratio of the upstream area to the slope, Niu et al. (2005)) is larger than or equal to the grid cell mean topographic index. It is the value of the discrete cumulative distribution function (CDF) of the topographic index when the grid cell mean water table depth is zero.

3605 A3.9 CABLE

The original CABLE model (version 2, Kowalczyk et al., 2013) generates surface runoff from excess infiltration only when the first three soil layers are at least 95% saturated. There is no other surface runoff

118

3608 generation process. However, Decker (2015) implemented subgrid-scale soil water content variability, 3609 explicit runoff generation and ground water in CABLE. The fraction of the saturated area, F_{sat} , follows 3610 Entekhabi and Eagleson (1989) and is defined as:

$$3611 F_{sat} = \int_{\kappa_n}^{\infty} f(s) ds [A50]$$

where f(s) is the Gamma-distribution of Eq. [42], and κ_p is defined by Eq. [A53]. One can solve this integral assuming a constant α_c in Eq. [42], which then links $s = \frac{\langle \theta \rangle - \langle \theta_r \rangle}{\langle \theta_s \rangle - \langle \theta_r \rangle}$, the mean of the vertically averaged relative saturation over the grid cell, with λ_s due to the properties of the Gamma-distribution (Eq. [42]):

$$3615 \qquad \lambda_s = \frac{1}{2s} \tag{A51}$$

3616 For $\alpha_c = \frac{1}{2}$, one gets:

3617
$$F_{sat} = 1 - erf\left(\sqrt{\frac{\kappa_p}{\lambda_s}}\right)$$
 [A52]

3618 Finally, κ_p is parameterized by an empirical formulation as:

3619
$$\kappa_p = C_v \sigma_{slope}$$
 [A53]

3620 with C_v as a fitting parameter and σ_{slope} as the standard deviation of the subgrid slope.

3621 Haverd et al. (2016) and Cuntz and Haverd (2018) recently implemented a new soil (Haverd and Cuntz,

2010b) and snow model with physically accurate freeze-thaw processes within CABLE, which is currentlycombined with the developments of (Decker, 2015).

3624 A3.10 SSiB

3625 In SSiB the model, the normalized runoff I_{roff} is spatially distributed as a function of fractional area 3626 of grid area x, (0 < x < 1) (Sato et al., 1989):

3627
$$I_{roff}(x) = a_{SSiB}e^{-b_{SSiB}x} + c_{SSiB}$$
 [A54]

where *a*_{SSiB}, *b*_{SSiB}, *c*_{SSiB} are constants. This distribution has also been applied to the convective precipitation. The constants (*a*, *b*, and *c*) were obtained by comparison with the observational data and are normalized so that:

3631
$$\int_{0}^{1} I_{roff}(x) dx = 1$$
 [A55]

Based the above two spatial distributions, the saturation fraction, F_{sat} , could be obtained (Sato et al., 1989) as:

3634
$$F_{sat} = \frac{1}{b_{SSiB}} \log \left(\frac{K_s \Delta t}{P_{drop} a_{SSiB}} \right) - \frac{c_{SSiB}}{a_{SSiB}}$$
[A56]

where K_s is the saturated hydraulic conductivity [L T⁻¹], Δt is time interval [T], and P_{drop} is the precipitation reaching the surface after interception by canopy [L T⁻¹]. The spatial distribution of convective precipitation has also been applied to obtained the P_{drop} (Sellers et al., 1996).

3638 A3.12 JSBACH

JSBACH uses the original Arno scheme (Dümenil and Todini, 1992) to determine surface runoff and infiltration. Accordingly, the saturated fraction is estimated for the grid box fraction for which soil water capacity of the rootzone is less than or equal to the gridbox mean rootzone soil moisture. The shape parameter *b* is being determined using Eq. [46].

3643 A3 Use of PTF for the estimation of K_s

For soils with low organic carbon content, Noah-MP, and CLM 4.5 use the PTFs developed on point scale by Clapp and Hornberger (1978) and Cosby et al. (1984) to estimate K_s . In ISBA-SURFEX, K_s is related to the soil textural properties (clay and sand) using the Noilhan and Lacarrère (1995) continuous relationships derived from theses PTFs. These PTFs are basically class PTFs (Van Looy et al., 2017) that give average values of Brooks Corey parameters and the measured K_s for each textural class of the USDA classification and are also developed on point scale.

Soil classes in CLSM are parameterized by Campbell (1974) equations and the corresponding hydraulic parameters including K_s are based on lookup tables for twelve different soil textural classes or using the PTFs of Wösten et al. (2001), which are both developed on point scale. Campbell's method used the Brooks-Corey parameterization of the soil water retention curve and a single point measurement of K at a given water content to calculate the complete hydraulic conductivity function.

None of the models directly considers the effect of soil structure on saturated hydraulic conductivity. Only the OLAM-SOIL considers implicitly the impact of structural properties on K_s by linearly interpolating between the measured K_s value and the value of the hydraulic conductivity obtained at a pressure head of about -6 cm as proposed by Weynants et al. (2009). Based on the work of Jarvis (2007) this value was
considered to delineate the saturation range that is controlled by structural properties.

3660 In JSBACH, K_s values are assigned to 11 textural classes based on data presented in Beringer et al. (2001). 3661 However, the origin of the tabulated K_s values that appear to be mean measured values for a specific 3662 textural class is not clear. Most likely, they were derived from the dataset of Clapp and Hornberger (1978).

3663 JULES uses sand and clay content to estimate the saturated hydraulic conductivity for the main soil 3664 column. Below the soil column is an additional `deep water store', within which K_s decreases exponentially 3665 with depth with a dampening factor set equal to 3 as proposed by Clark and Gedney (2008). K_s values can 3666 also be defined for each soil layer and can account for the presence of soil organic matter (Chadburn et 3667 al., 2015a). Rahman and Rosolem (2017) incorporated the effect of preferential flow into JULES (but note 3668 that this has not yet been adopted in the current 'official' UKMO version of JULES), to allow simulation of 3669 highly fractured unsaturated Chalk soils. Their bulk conductivity (BC) model introduces only two additional 3670 parameters (namely the macroporosity factor and the soil wetness threshold parameter for fracture flow 3671 activation) and uses the saturated hydraulic conductivity from the chalk matrix. The BC model was 3672 implemented into JULES and applied to a study area encompassing the Kennet catchment in the southern 3673 UK and the model performance at the catchment scale was evaluated against independent data sets (e.g., 3674 runoff and latent heat flux). The results demonstrated that the inclusion of the BC model in JULES 3675 improved the simulations of land surface water and energy fluxes over the chalk-dominated Kennet 3676 catchment. This simple approach to account for soil structure has potential for large-scale land surface 3677 modelling applications. ORCHIDEE uses VG soil parameters (K_s , n, α , θ_r , and θ_s) for each USDA class. In 3678 addition, a decay of K_s with depth is imposed (as also in JULES), as written in Appendix A2.7. With respect 3679 to the horizontal variability, ORCHIDEE uses an exponential PDF to describe horizontal heterogeneity.

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