



1 **Development and evaluation of a variably saturated flow model in the global**  
2 **E3SM Land Model (ELM) Version 1.0**

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16 **Abstract**

17 Improving global-scale model representations of coupled surface and groundwater  
18 hydrology is important for accurately simulating terrestrial processes and predicting  
19 climate change effects on water resources. Most existing land surface models,  
20 including the default E3SM Land Model (ELMv0), which we modify here, routinely  
21 employ different formulations for water transport in the vadose and pheratic zones.  
22 In this work, we developed the Variably Saturated Flow Model (VSFM) in ELMv1 to  
23 unify the treatment of soil hydrologic processes in the unsaturated and saturated  
24 zones. VSFM was tested on three benchmark problems and results were evaluated  
25 against observations and an existing benchmark model (PFLOTRAN). The ELMv1-  
26 VSFM's subsurface drainage parameter,  $f_d$ , was calibrated to match an  
27 observationally-constrained and spatially-explicit global water table depth (WTD)  
28 product. An optimal  $f_d$  was obtained for 79% of global  $1.9^0 \times 2.5^0$  gridcells, while the  
29 remaining 21% of global gridcells had predicted WTD deeper than the  
30 observationally-constrained estimate. Comparison with predictions using the default  
31  $f_d$  value demonstrated that calibration significantly improved prediction, primarily  
32 by allowing much deeper WTDs. Model evaluation using the International Land Model  
33 Benchmarking package (ILAMB) showed that improvements in WTD predictions did  
34 not degrade model skill for any other metrics. We evaluated the computational  
35 performance of the VSFM model and found that the model is about 30% more  
36 expensive than the default ELMv0 with an optimal processor layout.



## 37 **1 Introduction**

38 Groundwater, which accounts for 30% of freshwater reserves globally, is a vital  
39 human water resource. It is estimated that groundwater provides 20-30% of global  
40 freshwater withdrawals (Petra, 2009; Zektser and Evertt, 2004), and that irrigation  
41 accounts for ~70% of these withdrawals (Siebert et al., 2010). Climate change is  
42 expected to impact the quality and quantity of groundwater in the future (Alley,  
43 2001). As temporal variability of precipitation and surface water increases in the  
44 future due to climate change, reliance on groundwater as a source of fresh water for  
45 domestic, agriculture, and industrial use is expected to increase (Taylor et al., 2013).

46 Local environmental conditions modulate the impact of rainfall changes on  
47 groundwater resources. For example, high intensity precipitation in humid areas may  
48 lead to a decrease in groundwater recharge (due to higher surface runoff), while arid  
49 regions are expected to see gains in groundwater storage (as infiltrating water  
50 quickly travels deep into the ground before it can be lost to the atmosphere)  
51 (Kundzewicz and Doli, 2009). Although global climate models predict changes in  
52 precipitation over the next century (Marvel et al., 2017), few global models that  
53 participated in the recent Coupled Model Inter-comparison Project (CMIP5; Taylor et  
54 al. (2012)) were able to represent global groundwater dynamics accurately (e.g.  
55 Swenson and Lawrence (2014))

56 Modeling studies have also investigated impacts, at watershed to global scale, on  
57 future groundwater resources associated with land-use (LU) and land-cover (LC)  
58 change (Dams et al., 2008) and ground water pumping (Ferguson and Maxwell, 2012;  
59 Leng et al., 2015). Dams et al. (2008) predicted that LU changes would result in a small  
60 mean decrease in subsurface recharge and large spatial and temporal variability in  
61 groundwater depth for the Kleine Nete basin in Belgium. Ferguson and Maxwell  
62 (2012) concluded that groundwater-fed irrigation impacts on water exchanges with  
63 the atmosphere and groundwater resources can be comparable to those from a 2.5 °C  
64 increase in air temperature for the Little Washita basin in Oklahoma, USA. By  
65 performing global simulations of climate change scenarios using CLM4, Leng et al.  
66 (2015) concluded that the water source (i.e., surface or groundwater) used for



67 irrigation depletes the corresponding water source while increasing the storage of  
68 the other water source. Recently, Leng et al. (2017) showed that irrigation method  
69 (drip, sprinkler, or flood) has impacts on water balances and water use efficiency in  
70 global simulations.

71 Groundwater models are critical for developing understanding of  
72 groundwater systems and predicting impacts of climate change (Green et al., 2011;  
73 Kollet and Maxwell, 2008). Kollet and Maxwell (2008) identified critical zones, i.e.,  
74 regions within the watershed with water table depths between 1 – 5 m, where the  
75 influence of groundwater dynamics was largest on surface energy budgets. Numerical  
76 studies have demonstrated impacts of groundwater dynamics on several key Earth  
77 system processes, including soil moisture (Chen and Hu, 2004; Liang et al., 2003;  
78 Salvucci and Entekhabi, 1995; Yeh and Eltahir, 2005), runoff generation (Levine and  
79 Salvucci, 1999; Maxwell and Miller, 2005; Salvucci and Entekhabi, 1995; Shen et al.,  
80 2013), surface energy budgets (Alkhaier et al., 2012; Niu et al., 2017; Rihani et al.,  
81 2010; Soylyu et al., 2011), land-atmosphere interactions (Anyah et al., 2008; Jiang et  
82 al., 2009; Leung et al., 2011; Yuan et al., 2008), vegetation dynamics (Banks et al.,  
83 2011; Chen et al., 2010), and soil biogeochemistry (Lohse et al., 2009; Pacific et al.,  
84 2011).

85 Recognizing the importance of groundwater systems on terrestrial processes,  
86 groundwater models of varying complexity have been implemented in land surface  
87 models (LSMs) in recent years. Groundwater models in current LSMs can be classified  
88 into four categories based on their governing equations. Type-1 models assume a  
89 quasi-steady state equilibrium of the soil moisture profile above the water table  
90 (Hilberts et al., 2005; Koster et al., 2000; Walko et al., 2000). Type-2 models use a  $\theta$ -  
91 based (where  $\theta$  is the water volume content) Richards equation in the unsaturated  
92 zone coupled with a lumped unconfined aquifer model in the saturated zone.  
93 Examples of one-dimensional Type-2 models include Liang et al. (2003), Yeh and  
94 Eltahir (2005), Niu et al. (2007), and Zeng and Decker (2009). Examples of quasi  
95 three-dimensional Type-2 models are York et al. (2002); Fan et al. (2007); Miguez-  
96 Macho et al. (2007); and Shen et al. (2013). Type-3 models include a three-



97 dimensional representation of subsurface flow based on the variably saturated  
98 Richards equation (Maxwell and Miller, 2005; Tian et al., 2012). Type-3 models  
99 employ a unified treatment of hydrologic processes in the vadose and pheratic zones  
100 but lump changes associated with water density and unconfined aquifer porosity into  
101 a specific storage term. The fourth class (Type-4) of subsurface flow and reactive  
102 transport models (e.g., PFLOTRAN (Hammond and Lichtner, 2010), TOUGH2 (Pruess  
103 et al., 1999), and STOMP (White and STOMP, 2000)) combine a water equation of  
104 state (EoS) and soil compressibility with the variably saturated Richards equation.  
105 Type-4 models have not been routinely coupled with LSMs to address climate change  
106 relevant research questions.

107 The Energy, Exascale, Earth System Model (E3SM) is a new Earth System  
108 Modeling project sponsored by the U.S. Department of Energy (DOE). The E3SM  
109 model started from the Community Earth System Model (CESM) version 1\_3\_beta10  
110 (Oleson, 2013). Specifically, the initial version (v0) of the E3SM Land Model (ELM)  
111 was based off the Community Land Model's (CLM's) tag 4\_5\_71. ELMv0 uses a Type-  
112 2 subsurface hydrology model based on Zeng and Decker (2009). In this work, we  
113 developed in ELMv1 a Type-4 Variably Saturated Flow model (VSFM) to provide a  
114 unified treatment of soil hydrologic processes within the unsaturated and saturated  
115 zones. The VSFM formulation is based on the isothermal single phase flow model of  
116 PFLOTRAN (see Hammond and Lichtner (2010) for details regarding various modes  
117 supported in PFLOTRAN). While PFLOTRAN is a massively parallel, three-  
118 dimensional subsurface model, the VSFM is a serial, one-dimensional model that is  
119 appropriate for climate scale applications.

120 This paper is organized into several sections: (1) brief review of the ELMv0  
121 subsurface hydrology model; (2) overview of the VSFM formulation integrated in  
122 ELMv1; (3) application of the new model formulation to three benchmark problems;  
123 (4) development of a subsurface drainage parameterization necessary to predict  
124 global water table depths (WTDs) comparable to recently released observationally-  
125 constrained estimates; (5) comparison of ELMv1 global simulations with the default  
126 subsurface hydrology model and VSFM against multiple observations using the



127 International Land Model Benchmarking package (ILAMB; Hoffman et al. (2017));  
 128 and (6) a summary of major findings.

## 129 2 Methods

### 130 2.1 Current Model Formulation

131 Water flow in the unsaturated zone is often described by the  $\theta$ -based Richards  
 132 equation:

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot \mathbf{q} - Q \quad (1)$$

133

134 where  $\theta$  [ $\text{m}^3$  of water  $\text{m}^{-3}$  of soil] is the volumetric soil water content,  $t$  [s] is time,  $\mathbf{q}$   
 135 [ $\text{m s}^{-1}$ ] is the Darcy water flux, and  $Q$  [ $\text{m}^3$  of water  $\text{m}^{-3}$  of soil  $\text{s}^{-1}$ ] is a soil moisture  
 136 sink term. The Darcy flux,  $\vec{q}$ , is given by

$$\mathbf{q} = -K\nabla(\psi + z) \quad (2)$$

137 where  $K$  [ $\text{ms}^{-1}$ ] is the hydraulic conductivity,  $z$  [m] is height above some datum in the  
 138 soil column and  $\psi$  [m] is the soil matric potential. The hydraulic conductivity and soil  
 139 matric potential are modeled as non-linear function of volumetric soil moisture  
 140 following Clapp and Hornberger (1978):

$$K = \Theta_{ice} K_{sat} \left( \frac{\theta}{\theta_{sat}} \right)^{2B+3} \quad (3)$$

$$\psi = \psi_{sat} \left( \frac{\theta}{\theta_{sat}} \right)^{-B} \quad (4)$$

141

142 where  $K_{sat}$  [ $\text{m s}^{-1}$ ] is saturated hydraulic conductivity,  $\psi_{sat}$  [m] is saturated soil  
 143 matric potential,  $B$  is a linear function of percentage clay and organic content (Oleson,  
 144 2013), and  $\Theta_{ice}$  is the ice impedance factor (Swenson et al., 2012). ELMv0 uses the  
 145 modified form of Richards equation of Zeng and Decker (2009) that computes Darcy  
 146 flux as

$$\mathbf{q} = -K\nabla(\psi + z - C) \quad (5)$$

147 where  $C$  is a constant hydraulic potential above the water table,  $z_v$ , given as



$$C = \psi_E + z = \psi_{sat} \left( \frac{\theta_E(z)}{\theta_{sat}} \right)^{-B} = \psi_{sat} + z_v \quad (6)$$

148 where  $\psi_E$  [m] is the equilibrium soil matric potential,  $\theta_E$  [ $\text{m}^3 \text{m}^{-3}$ ] is volumetric soil  
 149 water content at equilibrium soil matric potential, and  $z_v$  [m] is height of water table  
 150 above the reference datum. ELMv0 uses a cell-centered finite volume spatial  
 151 discretization and backward Euler implicit time integration. By default, ELMv0's  
 152 vertical discretization of a soil column yields 15 soil layers of exponentially varying  
 153 soil thicknesses that reach a depth of 42.1 m Only the first 10 soils layers (or top 3.8  
 154 m of each soil column), are hydrologically active, while thermal processes are  
 155 resolved for all 15 soils layers. The nonlinear Darcy flux is linearized using Taylor  
 156 series expansion and the resulting tridiagonal system of equations is solved by LU  
 157 factorization.

158 Flow in the saturated zone is modeled as an unconfined aquifer below the soil  
 159 column based on the work of Niu et al. (2007). Exchange of water between the soil  
 160 column and unconfined aquifer depends on the location of the water table. When the  
 161 water table is below the last hydrologically active soil layer in the column, a recharge  
 162 flux from the last soil layer replenishes the unconfined aquifer. A zero-flux boundary  
 163 condition is applied to the last hydrologically active soil layer when the water table is  
 164 within the soil column. The unconfined aquifer is drained by a flux computed based  
 165 on the SIMTOP scheme of Niu et al. (2007) with modifications to account for frozen  
 166 soils (Oleson, 2013).

## 167 2.2 New VSFM Model Formulation

168 In the VSFM formulation integrated in ELMv1, we use the mass conservative form of  
 169 the variably saturated subsurface flow equation (Farthing et al., 2003; Hammond and  
 170 Lichtner, 2010; Kees and Miller, 2002):

$$\frac{\partial(\phi s_w \rho)}{\partial t} = -\nabla \cdot (\rho \mathbf{q}) - Q \quad (7)$$

171 where  $\phi$  [ $\text{m}^3 \text{m}^{-3}$ ] is the soil porosity,  $s_w$  [-] is saturation,  $\rho$  [ $\text{kg m}^{-3}$ ] is water density,  
 172  $\mathbf{q}$  [ $\text{m s}^{-1}$ ] is the Darcy velocity, and  $Q$  [ $\text{kg m}^{-3} \text{s}^{-1}$ ] is a water sink. We restrict our model



173 formulation to a one-dimensional system and the flow velocity is defined by Darcy's  
 174 law:

$$\mathbf{q} = -\frac{kk_r}{\mu} \nabla(P + \rho g z) \quad (8)$$

175 where  $k$  [m<sup>2</sup>] is intrinsic permeability,  $k_r$  [-] is relative permeability,  $\mu$  [Pa s] is  
 176 viscosity of water,  $P$  [Pa] is pressure,  $g$  [m s<sup>-2</sup>] is the acceleration due to gravity, and  
 177  $z$  [m] is elevation above some datum in the soil column.

178 In order to close the system, a constitutive relationship is used to express soil  
 179 saturation and relative permeability as a function of soil matric pressure. Analytic  
 180 Water Retention Curves (WRCs) are used to model effective saturation ( $s_e$ )

$$s_e = \left( \frac{s_w - s_r}{1 - s_r} \right) \quad (9)$$

181 where  $s_w$  is soil saturation and  $s_r$  is residual soil saturation. We have implemented  
 182 Brooks and Corey (1964) (equation 10) and van Genuchten (1980) (equation 11)  
 183 WRCs:

$$s_e = \begin{cases} \left( \frac{-P_c}{P_c^0} \right)^{-\lambda} & \text{if } P_c < 0 \\ 1 & \text{if } P_c \geq 0 \end{cases} \quad (10)$$

$$s_e = \begin{cases} [1 + (\alpha |P_c|^n)]^{-m} & \text{if } P_c < 0 \\ 1 & \text{if } P_c \geq 0 \end{cases} \quad (11)$$

184 where  $P_c$  [Pa] is the capillary pressure and  $P_c^0$  [Pa] is capillary pressure denoting air  
 185 entry point. The capillary pressure is computed as  $P_c = P - P_{ref}$  where  $P_{ref}$  is  $P_c^0$  for  
 186 Brooks and Corey WRC and typically the atmospheric pressure (=101,325 [Pa]) is  
 187 used for van Genuchten WRC. In addition, a smooth approximation of equation (10)  
 188 and (11) was developed to facilitate convergence of the nonlinear solver (Appendix  
 189 A). Relative soil permeability was modeled using the Mualem (1976) formulation:

$$\kappa_r(s_e) = \begin{cases} s_e^{0.5} \left[ 1 - \left( 1 - s_e^{1/m} \right)^m \right] & \text{if } P < P_{ref} \\ 1 & \text{if } P \geq P_{ref} \end{cases} \quad (12)$$

190 Lastly, we used an EoS for water given by Tanaka et al. (2001):

$$\rho(P, T) = [1 + (k_0 + k_1 T + k_2 T^2)(P - P_{ref})] a_5 \left[ 1 - \frac{(T + a_1)^2 (T + a_2)}{a_3 (T + a_4)} \right] \quad (13)$$



191 where

$$\begin{aligned}k_0 &= 50.74 \times 10^{-11} [\text{Pa}^{-1}] \\k_1 &= -0.326 \times 10^{-11} [\text{Pa}^{-1}\text{C}^{-1}] \\k_2 &= 0.00416 \times 10^{-11} [\text{Pa}^{-1}\text{C}^2] \\a_1 &= -3.983035 [\text{C}] \\a_2 &= 301.797 [\text{C}] \\a_3 &= 522558.9 [\text{C}^2] \\a_4 &= 69.34881 [\text{C}] \\a_5 &= 999.974950 [\text{kg m}^{-3}]\end{aligned}$$

192 Unlike the default subsurface hydrology model, the VSFM is applied over the  
193 full soil depth (in the default model, 15 soil layers). The VSFM model replaces both  
194 the  $\theta$ -based Richards equation and the unconfined aquifer of the default model. In the  
195 VSFM model, water table depth is diagnosed based on the vertical soil liquid pressure  
196 profile. Like the default model, drainage flux is computed based on the modified  
197 SIMTOP approach and is vertically distributed over the soil layers below the water  
198 table.

### 199 2.2.1 Discrete Equations

200 We use a cell-centered finite volume discretization to decompose the spatial  
201 domain,  $\Omega$ , into  $N$  non-overlapping control volumes,  $\Omega_n$ , such that  $\Omega = \cup_{n=1}^N \Omega_n$  and  $\Gamma_n$   
202 represents the boundary of the  $n$ -th control volume. Applying a finite volume integral  
203 to equation (7) and the divergence theorem yields

$$\frac{\partial}{\partial t} \int_{\Omega_n} (\phi s_w \rho) dV = - \int_{\Gamma_n} (\rho \mathbf{q}) \cdot d\mathbf{A} - \int_{\Omega_n} Q \quad (14)$$

204 The discretized form of the left hand side term and first term on the right hand side  
205 of equation (14) are approximated as:

206

$$\frac{\partial}{\partial t} \int_{\Omega_n} (\phi s_w \rho) dV \approx \left( \frac{d}{dt} (\phi s_w \rho) \right) V_n \quad (15)$$



$$\int_{\Gamma_n} (\rho \mathbf{q}) \cdot d\mathbf{A} \approx \sum_{n'} (\rho \mathbf{q})_{nn'} \cdot \mathbf{A}_{nn'} \quad (16)$$

207 After substituting equations (15) and (16) in equation (14), the resulting ordinary  
 208 differential equation for the variably saturated flow model is

$$\left( \frac{d}{dt} (\phi S_w \rho) \right) V_n = - \sum_{n'} (\rho \mathbf{q})_{nn'} \cdot \mathbf{A}_{nn'} - Q_n V_n \quad (17)$$

209 We perform temporal integration of equation (17) using the backward-Euler scheme:

$$\left( \frac{(\phi S_w \rho)_n^{t+1} - (\phi S_w \rho)_n^t}{\Delta t} \right) V_n = - \sum_{n'} (\rho \mathbf{q})_{nn'}^{t+1} \cdot \mathbf{A}_{nn'} - Q_n^{t+1} V_n \quad (18)$$

210 Rearranging terms of equation (18) results in a nonlinear equation for the unknown  
 211 pressure at timestep  $t + 1$  as

$$\left( \frac{(\phi S_w \rho)_n^{t+1} - (\phi S_w \rho)_n^t}{\Delta t} \right) V_n + \sum_{n'} (\rho \mathbf{q})_{nn'}^{t+1} \cdot \mathbf{A}_{nn'} + Q_n^{t+1} V_n = 0 \quad (19)$$

212 In this work, we find the solution to the system of nonlinear equations given by  
 213 equation (19) using Newton's method with the Portable, Extensible Toolkit for  
 214 Scientific Computing (PETSc) library (Balay et al., 2016). PETSc provides a suite of  
 215 data structures and routines for the scalable solution of partial differential equations.  
 216 A Smooth approximation of the Brooks and Corey (1964) (SBC) water retention curve  
 217 was developed to facilitate faster convergence of the nonlinear solver (Appendix A).

### 218 2.3 VFSM single-column evaluation

219 We tested the VFSM with three idealized 1-dimensional test problems. First, the  
 220 widely studied problem for 1D Richards equation of infiltration in dry soil by Celia et  
 221 al. (1990) was used. The problem setup consists of a 1.0 m long soil column with a  
 222 uniform initial pressure of  $-10.0$  m (= 3535.5 Pa). Time invariant boundary  
 223 conditions applied at the top and bottom of soil column are  $-0.75$  m (= 9399.1 Pa)  
 224 and  $-10.0$  m (= 3535.5 Pa), respectively. The soil properties for this test are given in  
 225 Table 1. A vertical discretization of 0.01 m is used in this simulation.

226 Second, we simulated transient one-dimensional vertical infiltration in two-  
 227 layered soil system as described in Srivastava and Yeh (1991). The domain consisted



228 of a 2 m tall soil column divided equally in two soil types. Except soil permeability, all  
229 other soil properties of the two soil types are the same. The bottom soil is 10 times  
230 less permeable than the top (Table1). Unlike Srivastava and Yeh (1991), who used  
231 exponential functions of soil liquid pressure to compute hydraulic conductivity and  
232 soil saturation, we used Mualem (1976) and van Genuchten (1980) constitutive  
233 relationships. Since our choice of constitutive relationships for this setup resulted in  
234 absence of an analytical solution, we compared VSFM simulations against PFLOTRAN  
235 results. The domain was discretized in 200 control volumes of equal soil thickness.  
236 Two scenarios, wetting and drying, were modeled to test the robustness of the VSFM  
237 solver robustness. Initial conditions for each scenario included a time invariant  
238 boundary condition of 0 m (=  $1.01325 \times 10^5$  Pa) for the lowest control volume and a  
239 constant flux of  $0.9 \text{ cm hr}^{-1}$  and  $0.1 \text{ cm hr}^{-1}$  at the soil surface for wetting and drying  
240 scenarios, respectively.

241 Third, we compare VSFM and PFLOTRAN predictions for soil under variably  
242 saturated conditions. The 1-dimensional 1 m deep soil column was discretized in 100  
243 equal thickness control volumes. A hydrostatic initial condition was applied such that  
244 water table is 0.5 m below the soil surface. A time invariant flux of  $2.5 \times 10^{-5} \text{ m s}^{-1}$  is  
245 applied at the surface, while the lowest control volume has a boundary condition  
246 corresponding to the initial pressure value at the lowest soil layer. The soil properties  
247 used in this test are the same as those used in the first evaluation.

#### 248 **2.4 Global Simulations and groundwater depth analysis**

249 We performed global simulations with ELMv1-VSFM at a spatial resolution of  
250  $1.9^0$  (latitude)  $\times$   $2.5^0$  (longitude) with a 30 [min] time-step for 200 years, including a  
251 180 year spinup and the last 20 years for analysis. The simulations were driven by  
252 CRUNCEP meteorological forcing from 1991-2010 (Piao et al., 2012) and configured  
253 to use prescribed satellite phenology.

254 For evaluation and calibration, we used the Fan et al. (2013) global  $\sim 1$  km  
255 horizontal resolution WTD dataset (hereafter F2013 dataset), which is based on a  
256 combination of observations and hydrologic modeling. We aggregated the dataset to  
257 the ELMv1-VSFM spatial resolution. ELM-VSFM's default vertical soil discretization



258 uses 15 soil layers to a depth of  $\sim 42$  m, with an exponentially varying soil thickness.  
259 However,  $\sim 13\%$  of F2013 land gridcells have a water table deeper than 42 m. We  
260 therefore modified ELMv1-VSFM to extend the soil column to a depth of 150 m with  
261 59 soil layers; the first nine soil layer thicknesses were the same as described in  
262 Oleson (2013) and the remaining layers (10-59) were set to a thickness of 3 m.

## 263 2.5 Estimation of the subsurface drainage parameterization

264 In the VSFM formulation, the dominant control on long-term GW depth is the  
265 subsurface drainage flux,  $q_d$  [ $\text{kg m}^{-2} \text{s}^{-1}$ ], which is calculated based on water table  
266 depth,  $z_v$  [m], (Niu et al. (2005)):

$$q_d = q_{d,max} \exp(-f_d z_v) \quad (20)$$

267 where  $q_{d,max}$  [ $\text{kg m}^{-2} \text{s}^{-1}$ ] is the maximum drainage flux that depends on gridcell slope  
268 and  $f_d$  [ $\text{m}^{-1}$ ] is an empirically-derived parameter. The subsurface drainage flux  
269 formulation of Niu et al. (2005) is similar to the TOPMODEL formulation (Beven and  
270 Kirkby, 1979) and assumes the water table is parallel to the soil surface. While  
271 Sivapalan et al. (1987) derived  $q_{d,max}$  as a function of lateral hydraulic anisotropy,  
272 hydraulic conductivity, topographic index, and decay factor controlling vertical  
273 saturated hydraulic conductivity, Niu et al. (2005) defined  $q_{d,max}$  as a single  
274 calibration parameter. ELMv0 uses  $f_d = 2.5 \text{ m}^{-1}$  as a global constant and estimates  
275 maximum drainage flux when WTD is at the surface as  $q_{d,max} = 10 \sin(\beta) \text{ kg m}^{-2} \text{ s}^{-1}$ .  
276 Of the two parameters,  $f_d$  and  $q_{d,max}$ , available for model calibration, we choose to  
277 calibrate  $f_d$  because the uncertainty analysis by Hou et al. (2012) identified it as the  
278 most significant hydrologic parameter in CLM4. To improve on the  $f_d$  parameter  
279 values, we performed an ensemble of global simulations with  $f_d$  values of 0.1, 0.2, 0.5,  
280 1.0, 2.5, 5.0, 10.0, and 20  $\text{m}^{-1}$ . Each ensemble simulation was run for 200 years to  
281 ensure an equilibrium solution, and the last 20 years were used for analysis. A non-  
282 linear functional relationship between  $f_d$  and WTD was developed for each gridcell  
283 and then the F2013 dataset was used to estimate an optimal  $f_d$  for each gridcell.



## 284 **2.6 Global ELM-VSFM evaluation**

285 With the optimal  $f_d$  values, we ran a ELM-VSFM simulation using the protocol  
286 described above. We then used the International Land Model Benchmarking package  
287 (ILAMB) to evaluate the ELMv1-VSFM predictions of surface energy budget, total  
288 water storage anomalies (TWSA), and river discharge. ILAMB evaluates model  
289 prediction bias, RMSE, and seasonal and diurnal phasing against multiple  
290 observations of energy, water, and carbon cycles at in-situ, regional, and global scales.  
291 Since ELM-VSFM simulations in this study did not include an active carbon cycle, we  
292 used the following ILAMB benchmarks for water and energy cycles: (i) latent and  
293 surface energy fluxes using site-level measurements from FLUXNET (Lasslop et al.,  
294 2010) and globally from FLUXNET-MTE (Jung et al., 2009)); (ii) terrestrial water  
295 storage anomaly (TWSA) from the Gravity Recovery And Climate Experiment  
296 (GRACE) observations (Kim et al., 2009); and (iii) stream flow for the 50 largest global  
297 river basins (Dai and Trenberth, 2002). We applied ILAMB benchmarks for ELMv1-  
298 VSFM simulations with default and calibrated  $f_d$  to ensure improvements in WTD  
299 predictions did not degrade model skill for other processes.

## 300 **3 Results and discussion**

### 301 **3.1 VSFM single-column evaluation**

302 For the 1D Richards equation infiltration in dry soil comparison, we evaluated  
303 the solutions at 24-hr against those published by Celia et al. (1990) (Figure 1). The  
304 VSFM solver accurately represented the sharp wetting front over time, where soil  
305 hydraulic properties change dramatically due to non-linearity in the soil water  
306 retention curve.

307 For the model evaluation of infiltration and drying in layered soil, the results of  
308 the VSFM and PFLOTRAN are essentially identical. In both models and scenarios, the  
309 higher permeability top soil responds rapidly to changes in the top boundary  
310 condition and the wetting and drying fronts progressively travel through the less



311 permeable soil layer until soil liquid pressure in the entire column reaches a new  
312 steady state by about 100 h (Figure 2).

313 We also evaluated the VSFM predicted water table dynamics against PFLOTRAN  
314 predictions from an initial condition of saturated soil below 0.5 m depth. The  
315 simulated water table rises to 0.3 m depth by 1 day and reaches the surface by 2 days,  
316 and the VSFM and PFLOTRAN predictions are essentially identical Figure 3. These  
317 three evaluation simulations demonstrate the VSFM accurately represents soil  
318 moisture dynamics under conditions relevant to ESM-scale prediction.

### 319 **3.2 Subsurface drainage parameterization estimation**

320 The simulated nonlinear WTD- $f_d$  relationship is a result of the subsurface  
321 drainage parameterization flux given by equation (20) (Figure 4(a) and (b)). For  
322  $0.1 \leq f_d \leq 1$ , the slope of the WTD- $f_d$  relationship for all gridcells is log-log linear  
323 with a slope of  $-1.0 \pm 0.1$ . The log-log linear relationship breaks down for  $f_d > 1$ ,  
324 where the drainage flux becomes much smaller than infiltration and  
325 evapotranspiration (Figure 4(c) and (d)). Thus, at larger  $f_d$ , the steady state  $z_{\nabla}$   
326 becomes independent of  $f_d$  and is determined by the balance of infiltration and  
327 evapotranspiration.

328 For 79% of the global gridcells, the ensemble range of simulated WTD spanned  
329 the F2013 dataset. The optimal value of  $f_d$  for each of these gridcells was obtained by  
330 linear interpolation in the log-log space (e.g., Figure 4 (a)). For the remaining 21% of  
331 gridcells where the shallowest simulated WTD across the range of  $f_d$  was deeper than  
332 that in the F2013 dataset, the optimal  $f_d$  value was chosen as the one that resulted in  
333 the lowest absolute WTD error (e.g., Figure 4 (b)). At large  $f_d$  values, the drainage flux  
334 has negligible effect on WTD, yet simulated WTD is not sufficiently shallow to match  
335 the F2013 observations, which indicates that either evapotranspiration is too large  
336 or infiltration is too small. There was no difference in the mean percentage of sand  
337 and clay content between grids cells with and without an optimal  $f_d$  value. The  
338 optimal  $f_d$  has a global average of  $1.60 \text{ m}^{-1} \pm 2.68 \text{ m}^{-1}$  and 72% of global gridcells have  
339 an optimal  $f_d$  value lower than the global average (Figure 5).



### 340 3.3 Global simulation evaluation

341 The ELMv1-VSFM predictions are much closer to the F2013 dataset (Figure 6a)  
342 using optimal globally-distributed  $f_d$  values (Figure 6c) compared to the default  $f_d$   
343 value (Figure 6b). The significant reduction in WTD bias (model – observation) is  
344 mostly due to improvement in the model’s ability to accurately predict deep WTD  
345 using optimal  $f_d$  values. In the simulation using optimal globally-distributed  $f_d$   
346 values, all gridcells with WTD bias > 3.7 m were those for which an optimal  $f_d$  was  
347 not found. The mean global bias, RMSE, and  $R^2$  values were all improved in the new  
348 ELMv1-VSFM compared to the default model (Table 1). The 79% of global grid cells  
349 for which an optimal  $f_d$  value was estimated had significantly better water table  
350 prediction with a bias, RMSE, and  $R^2$  of -0.04 m, 0.67m, and 0.99, respectively, as  
351 compared to the remaining 21% of global grid that had a bias, RMSE, and  $R^2$  of -9.82  
352 m, 18.08m, and 0.31, respectively. The simulated annual WTD range, which we define  
353 to be the difference between maximum and minimum WTD in a year, has a spatial  
354 mean and standard deviation of 0.32 m and 0.58 m, respectively, using optimal  $f_d$   
355 values (Figure 7 (a)). The annual WTD range decreased by 0.24 m for the 79% of the  
356 grid cells for which an optimal  $f_d$  value was estimated (Figure 7 (b)).

357 Globally-averaged WTD in ELMv1-VSFM simulations with default  $f_d$  and  
358 optimal  $f_d$  values were 10.5 m and 20.1 m, respectively. Accurate prediction of deep  
359 WTD in the simulation with optimal  $f_d$  caused very small differences in near-surface  
360 soil moisture (Figure 8). The 79% of grid cells with an optimal  $f_d$  value had deeper  
361 globally-averaged WTDs than when using the default  $f_d$  value (24.3 m vs. 8.6 m). For  
362 these 79% of grid cells, the WTD was originally deep enough to not impact near-  
363 surface conditions (Kollet and Maxwell, 2008); therefore, further lowering of WTD  
364 led to negligible changes in near-surface hydrological conditions.

365 The International Land Model Benchmarking (ILAMB) package (Hoffman et al.,  
366 2017) provides a comprehensive evaluation of predictions of carbon cycle states and  
367 fluxes, hydrology, surface energy budgets, and functional relationships by  
368 comparison to a wide range of observations. We used ILAMB to evaluate the  
369 hydrologic and surface energy budget predictions from the new ELMv1-VSFM model



370 (Table 2). Optimal  $f_d$  values had inconsequential impacts on simulated surface  
371 energy fluxes at site-level and global scales. Optimal  $f_d$  values led to improvement in  
372 prediction of deep WTD (with a mean value of 24.3 m) for grid cells that had an  
373 average WTD of 8.7 m in the simulation using default  $f_d$  values. Thus, negligible  
374 differences in surface energy fluxes between the two simulations are consistent with  
375 the findings of Kollet and Maxwell (2008), who identified decoupling of groundwater  
376 dynamics and surface processes at a WTD of  $\sim 10$  m. There were slight changes in bias  
377 and RMSE for predicted TWSA, but the ILAMB score remained unchanged. The TWSA  
378 amplitude is lower for the simulation with optimal  $f_d$  values, consistent with the  
379 associated decrease in annual WTD range. ELM's skill in simulating runoff for the 50  
380 largest global watersheds remained unchanged.

381 Finally, we evaluated the computational costs of implementing VSFM in ELM,  
382 and compared them to the default model. We performed 5-years long simulations for  
383 default and VSFM using 96, 192, 384, 768, and 1536 cores on the Edison  
384 supercomputer at the National Energy Research Scientific Computing Center. Using  
385 an optimal processor layout, we found that ELMv1-VSFM is  $\sim 30\%$  more expensive  
386 than the default ELMv1 model

### 387 **3.4 Caveats and Future Work**

388 The significant improvement in WTD prediction using optimal  $f_d$  values  
389 demonstrates VSFM's capabilities to model hydrologic processes using a unified  
390 physics formulation for unsaturated-saturated zones. However, several caveats  
391 remain due to uncertainties in model structure, model parameterizations, and climate  
392 forcing data.

393 In this study, we assumed a spatially homogeneous depth to bedrock (DTB) of  
394 150 m. Recently, Brunke et al. (2016) incorporated a global  $\sim 1$  km dataset of soil  
395 thickness and sedimentary deposits (Pelletier et al., 2016) in CLM4.5 to study the  
396 impacts of soil thickness spatial heterogeneity on simulated hydrological and thermal  
397 processes. While inclusion of heterogeneous DTB in CLM4.5 added more realism to  
398 the simulation setup, no significant changes in simulated hydrologic and energy  
399 fluxes were reported by Brunke et al. (2016). Presently, work is ongoing in the E3SM



400 project to include variable DTB within ELM and future simulations will examine the  
401 impact of those changes on VFSM's prediction of WTD. Our use of the 'satellite  
402 phenology' mode, which prescribes transient LAI profiles for each plant functional  
403 type in the gridcell, ignored the likely influence of water cycle dynamics and nutrient  
404 constraints on the C cycle (Ghimire et al., 2016; Zhu et al., 2016).

405 Lateral water redistribution impacts soil moisture dynamics (Bernhardt et al.,  
406 2012), biogeochemical processes in the root zone (Grant et al., 2015), distribution of  
407 vegetation structure (Hwang et al., 2012), and land-atmosphere interactions (Chen  
408 and Kumar, 2001; Rihani et al., 2010). The ELMv1-VSMF developed in this study does  
409 not include lateral water redistribution between soil columns and only simulates  
410 vertical water transport. Lateral subsurface processes can be included in LSMs via a  
411 range of numerical discretization approaches of varying complexity, e.g., adding  
412 lateral water as source/sink terms in the 1D model, implementing an operator split  
413 approach to solve vertical and lateral processes in a non-iterative approach (Ji et al.,  
414 2017), or solving a fully coupled 3D model (Bisht et al., 2017; Bisht et al., 2018; Kollet  
415 and Maxwell, 2008). Additionally, lateral transport of water can be implemented in  
416 LSMs at a subgrid level (Milly et al., 2014) or grid cell level (Miguez-Macho et al.,  
417 2007). The current implementation of VFSM is such that each processor solves the  
418 variably saturated Richards equation for all independent soil columns as one single  
419 problem. Thus, extension of VFSM to solve the tightly coupled 3D Richards equation  
420 on each processor locally while accounting for lateral transport of water within grid  
421 cells and among grid cells is straightforward. The current VFSM implementation can  
422 also be easily extended to account for subsurface transport of water among grid cells  
423 that are distributed across multiple processors by modeling lateral flow as a  
424 source/sink in the 1D model. Tradeoffs between approaches to represent lateral  
425 processes and computational costs need to be carefully studied before developing  
426 quasi or fully three-dimensional land surface models.



## 427 **4 Summary and Conclusion**

428 Starting from the climate-scale land model ELMv0, we incorporated a unified  
 429 physics formulation to represent soil moisture and groundwater dynamics that are  
 430 solved using PETSc. Application of VSFM to three benchmarks problems  
 431 demonstrated its robustness to simulated subsurface hydrologic processes in  
 432 coupled unsaturated and saturated zones. Ensemble global simulations at  $1.9^0 \times 2.5^0$   
 433 were performed for 200 years to obtain spatially heterogeneous estimate of a  
 434 subsurface drainage parameter,  $f_d$ , that minimized the mismatch between predicted  
 435 and observed WTD. In order to simulated the deepest water table reported in the Fan  
 436 et al. (2013) dataset, we used 59 vertical soil layers that reached a depth of 150 m.

437 An optimal  $f_d$  was obtained for 79% of the grids cells in the domain. For the  
 438 remaining 21% of grid cells, simulated WTD always remained deeper than observed.  
 439 Calibration of  $f_d$  significantly improved global WTD prediction by reducing bias and  
 440 RMSE and increasing  $R^2$ . Grids without an optimal  $f_d$  were the largest contributor of  
 441 error in WTD predication. ILAMB benchmarks on simulations with default and  
 442 optimal  $f_d$  showed negligible changes to surface energy fluxes, TWSA, and runoff.  
 443 ILABM metrics ensured that model skill was not adversely impacted for all other  
 444 processes when optimal  $f_d$  values were used to improve WTD prediction.

445

## 446 **5 Appendix**

### 447 **5.1 Smooth approximation of Brooks-Corey water retention curve**

448 The Brooks and Corey (1964) water retention curve of equation (10) has a  
 449 discontinuous derivative at  $P = P_c^0$ . Figure A 1 shown an example. To improve  
 450 convergence of the nonlinear solver at small capillary pressures, the smoothed  
 451 Brooks-Corey function introduces a cubic polynomial,  $B(P_c)$ , in the neighborhood of  
 452  $P_c^0$ .

$$s_e = \begin{cases} (-\alpha P_c)^{-\lambda} & \text{if } P_c \leq P_u \\ B(P_c) & \text{if } P_u < P_c < P_s \\ 1 & \text{if } P_s \leq P_c \end{cases} \quad (21)$$



453 where the breakpoints  $P_u$  and  $P_s$  satisfy  $P_u < P_c^0 < P_s \leq 0$ . The smoothing  
 454 polynomial

$$B(P_c) = b_0 + b_1(P_c - P_s) + b_2(P_c - P_s)^2 + b_3(P_c - P_s)^3 \quad (22)$$

455 introduces four more parameters, whose values follow from continuity. In particular  
 456 matching the saturated region requires  $B(P_s) = b_0 = 1$ , and a continuous derivative  
 457 at  $P_c = P_s$  requires  $B'(P_s) = b_1 = 0$ . Similarly, matching the value and derivative at  
 458  $P_c = P_u$  requires

$$b_2 = \frac{-1}{\Delta^2} \left[ 3 - (\alpha P_u)^{-\lambda} \left( 3 + \frac{\lambda \Delta}{P_u} \right) \right] \quad (23)$$

$$b_3 = \frac{-1}{\Delta^3} \left[ 2 - (\alpha P_u)^{-\lambda} \left( 2 + \frac{\lambda \Delta}{P_u} \right) \right] \quad (24)$$

459 where  $\Delta = P_u - P_s$ . Note  $P_u \leq \Delta < 0$ .

460 In practice, setting  $P_u$  too close to  $P_c^0$  can produce an unwanted local maximum  
 461 in the cubic smoothing regime, resulting in  $s_e > 1$ . Avoiding this condition requires  
 462 that  $B(P_c)$  increase monotonically from  $P_c = P_u$ , where  $B'(P_c) > 0$ , to  $P_c = P_s$ , where  
 463  $B'(P_c) = 0$ . Thus a satisfactory pair of breakpoints ensures

$$B'(P_c) = [P_c - P_s][2b_2 + 3b_3(P_c - P_s)] > 0 \quad (25)$$

464 throughout  $P_u \leq P_c < P_s$ .

465 Let  $P_c^*$  denote a local extremum of  $B$ , so that  $B'(P_c^*) = 0$ . If  $P_c^* \neq P_s$ , it follows  
 466  $P_c^* - P_s = -2b_2/(3b_3)$ . Rewriting equation 22,  $B'(P_c) = (P_c - P_s)3b_3(P_c - P_c^*)$  shows  
 467 that  $B'(P_c^*) > 0$  requires either: (1)  $b_3 < 0$  and  $P_c^* < P_u$ ; or (2)  $b_3 > 0$  and  $P_c^* > P_u$ .  
 468 The first possibility places  $P_c^*$  outside the cubic smoothing regime, and so does not  
 469 constrain the choice of  $P_u$  or  $P_s$ . The second possibility allows an unwanted local  
 470 extremum at  $P_u < P_c^* < P_s$ . In this case,  $b_3 > 0$  implies  $b_2 < 0$  (since  $P_c^* < P_s \leq 0$ ).  
 471 Then since  $B''(P_c^*) = -2b_2$ , the local extremum is a maximum, resulting in  $s_e(P_c^*) >$   
 472 1.

473 Given a breakpoint  $P_s$ , one strategy for choosing  $P_u$  is to guess a value, then  
 474 check whether the resulting  $b_2$  and  $b_3$  produces  $P_u < P_c^* < P_s$ . If so,  $P_u$  should be  
 475 made more negative. An alternative strategy is to choose  $P_u$  in order the guarantee  
 476 acceptable values for  $b_2$  and  $b_3$ . One convenient choice forces  $b_2 = 0$ . Another picks  
 477  $P_u$  in order to force  $b_3 = 0$ . Both of these reductions: (1) ensure  $B(P_c)$  has a positive



478 slope throughout the smoothing interval; (2) slightly reduce the computation cost of  
 479 finding  $s_e(P_c)$  for  $P_c$  on the smoothing interval; and (3) significantly reduce the  
 480 computational cost of inverting the model, in order to find  $P_c$  as a function of  $s_e$ .

481 As shown in Figure A 1, the two reductions differ mainly in that setting  $b_2 = 0$   
 482 seems to produce narrower smoothing regions (probably due to the fact that this  
 483 choice gives zero curvature at  $P_c = P_s$ , while  $b_3 = 0$  yields a negative second  
 484 derivative there). However, we have not verified this observation analytically.

485 Both reductions require solving a nonlinear expression either equation (23) or  
 486 (24), for  $P_u$ . While details are beyond the scope of this paper, we note that we have  
 487 used a bracketed Newton-Raphson's method. The search switches to bisection when  
 488 Newton-Raphson would jump outside the bounds established by previous iterations,  
 489 and by the requirement  $P_u < P_c^0$ . In any event, since the result of this calculation may  
 490 be cached for use throughout the simulation, it need not be particularly efficient.

## 491 5.2 Residual equation of VSFM formulation

492 The residual equation for the VSFM formulation at  $t + 1$  time level for  $n$ -th control  
 493 volume is given by

$$R_n^{t+1} \equiv \left( \frac{(\phi s_w \rho)_n^{t+1} - (\phi s_w \rho)_n^t}{\Delta t} \right) V_n + \sum_{n'} (\rho \mathbf{q})_{nn'}^{t+1} \cdot \mathbf{A}_{nn'} + Q_n^{t+1} V_n = 0 \quad (26)$$

494 where  $\phi$  [mm<sup>3</sup> mm<sup>-3</sup>] is the soil porosity,  $s_w$  [-] is saturation,  $\rho$  [kg m<sup>-3</sup>] is water  
 495 density,  $\vec{q}_{nn'}$  [m s<sup>-1</sup>] is the Darcy flow velocity between  $n$ -th and  $n'$ -th control  
 496 volumes,  $A_{nn'}$  [m<sup>2</sup>] is the interface face area between  $n$ -th and  $n'$ -th control  
 497 volumes  $Q$  [kg m<sup>-3</sup> s<sup>-1</sup>] is a sink of water. The Darcy velocity is computed as

$$\mathbf{q}_{nn'} = - \left( \frac{\kappa \kappa_r}{\mu} \right)_{nn'} \left[ \frac{P_{n'} - P_n - \rho_{nn'} (\mathbf{g} \cdot \mathbf{d}_{nn'})}{d_n + d_{n'}} \right] \mathbf{n}_{nn'} \quad (27)$$

498 where  $\kappa$  [m<sup>2</sup>] is intrinsic permeability,  $\kappa_r$  [-] is relative permeability,  $\mu$  [Pa s] is  
 499 viscosity of water,  $P$  [Pa] is pressure,  $\mathbf{g}$  [m s<sup>-2</sup>] is the acceleration due to gravity,  
 500  $d_n$  [m] and  $d_{n'}$  [m] is distance between centroid of  $n$ -th and  $n'$ -th control volume to  
 501 the common interface between the two control volumes,  $\mathbf{d}_{nn'}$  is a distance vector  
 502 joining centroid of  $n$ -th and  $n'$ -th control volume, and  $\mathbf{n}_{nn'}$  is a unit normal vector  
 503 joining centroid of  $n$ -th and  $n'$ -th control volume.



504 The density at the interface of control volume,  $\rho_{nn'}$ , is computed as inverse  
 505 distance weighted average by

$$\rho_{nn'} = \omega_{n'}\rho_n + \omega_n\rho_{n'} \quad (28)$$

506 where  $\omega_n$  and  $\omega_{n'}$  are given by

$$\omega_n = \frac{d_n}{d_n + d_{n'}} = (1 - \omega_{n'}) \quad (29)$$

507 The first term on the RHS of equation 27 is computed as the product of distance  
 508 weighted harmonic average of intrinsic permeability,  $k_{nn'}$ , and upwinding of  
 509  $k_r/\mu$  ( $= \lambda$ ) as

$$\left(\frac{k k_r}{\mu}\right)_{nn'} = k_{nn'} \left(\frac{k_r}{\mu}\right)_{nn'} = \left[\frac{k_n k_{n'} (d_n + d_{n'})}{k_n d_{n'} + k_{n'} d_n}\right] \lambda_{nn'} \quad (30)$$

510 where

$$\lambda_{nn'} = \begin{cases} (k_r/\mu)_n & \text{if } \vec{q}_{nn'} > 0 \\ (k_r/\mu)_{n'} & \text{otherwise} \end{cases} \quad (31)$$

511 By substituting equation 28, 29 and 30 in equation 27, we obtain

$$\mathbf{q}_{nn'} = - \left[\frac{k_n k_{n'}}{k_n d_{n'} + k_{n'} d_n}\right] \lambda_{nn'} [P_{n'} - P_n - \rho_{nn'}(\mathbf{g} \cdot \mathbf{d}_{nn'})] \mathbf{n}_{nn'} \quad (32)$$

512

### 513 5.3 Jacobian equation of VSFM formulation

514 The discretized equations of VSFM leads to a system of nonlinear equations given by  
 515  $\mathbf{R}^{t+1}(\mathbf{P}^{t+1}) = \mathbf{0}$ , which are solved using Newton's method using the Portable,  
 516 Extensible Toolkit for Scientific Computing (PETSc) library. The algorithm of  
 517 Newton's method requires solution of the following linear problem

$$\mathbf{J}^{t+1,k}(\mathbf{P}^{t+1,k}) \Delta \mathbf{P}^{t+1,k} = -\mathbf{R}^{t+1,k}(\mathbf{P}^{t+1,k}) \quad (33)$$

518 where  $\mathbf{J}^{t+1,k}(\mathbf{P}^{t+1,k})$  is the Jacobian matrix. In VSFM, the Jacobian matrix is  
 519 computed analytically. The contribution to the diagonal and off-diagonal entry of the  
 520 Jacobian matrix from  $n$ -th residual equations are given by

$$J_{nn} = \frac{\partial R_n}{\partial P_n} = \left(\frac{V_n}{\Delta t}\right) \frac{\partial(\rho \phi s_w)}{\partial P_n} + \sum_{n'} \frac{\partial(\rho \mathbf{q})_{nn'}}{\partial P_n} A_{nn'} + \frac{\partial Q_n^{t+1}}{\partial P_n} V_n \quad (34)$$



$$J_{nn'} = \frac{\partial R_n}{\partial P_{n'}} = \sum_{n'} \frac{\partial(\rho \mathbf{q})_{nn'}}{\partial P_{n'}} \mathbf{A}_{nn'} + \frac{\partial Q_n^{t+1}}{\partial P_{n'}} V_n \quad (35)$$

521 The derivative of the accumulation term in  $J_{nn}$  is computed as

$$\frac{\partial(\rho \phi s_w)}{\partial P_n} = \phi s_w \frac{\partial \rho}{\partial P_n} + \rho s_w \frac{\partial \phi}{\partial P_n} + \rho \phi \frac{\partial s_w}{\partial P_n} \quad (36)$$

522 The derivative of flux between  $n$ -th and  $n'$ -th control volume with respect to  
 523 pressure of each control volume is given as

$$\frac{\partial(\rho \mathbf{q})_{nn'}}{\partial P_n} = \rho_{nn'} \frac{\partial \mathbf{q}_{nn'}}{\partial P_n} + \mathbf{q}_{nn'} \omega_n \frac{\partial \rho_n}{\partial P_n} \quad (37)$$

524

$$\frac{\partial(\rho \mathbf{q})_{nn'}}{\partial P_{n'}} = \rho_{nn'} \frac{\partial \mathbf{q}_{nn'}}{\partial P_{n'}} + \mathbf{q}_{nn'} \omega_{n'} \frac{\partial \rho_{n'}}{\partial P_{n'}} \quad (38)$$

525 Lastly, the derivative of Darcy velocity between  $n$ -th and  $n'$ -th control volume with  
 526 respect to pressure of each control volume is given as

$$\frac{\partial \mathbf{q}_{nn'}}{\partial P_n} = \left[ \frac{k_n k_{n'}}{k_n d_{n'} + k_{n'} d_n} \right] \lambda_{nn'} \left[ 1 + \omega_n (\mathbf{g} \cdot \mathbf{d}_{nn'}) \frac{\partial \rho_n}{\partial P_n} \right] \mathbf{n}_{nn'} + \mathbf{q}_{nn'} \frac{\partial(\ln(\lambda_{nn'}))}{\partial P_n} \quad (39)$$

$$\begin{aligned} \frac{\partial \mathbf{q}_{nn'}}{\partial P_{n'}} &= \left[ \frac{k_n k_{n'}}{k_n d_{n'} + k_{n'} d_n} \right] \lambda_{nn'} \left[ -1 + \omega_n (\mathbf{g} \cdot \mathbf{d}_{nn'}) \frac{\partial \rho_{n'}}{\partial P_{n'}} \right] \mathbf{n}_{nn'} \\ &+ \mathbf{q}_{nn'} \frac{\partial(\ln(\lambda_{nn'}))}{\partial P_{n'}} \end{aligned} \quad (40)$$

527

## 528 **6 Code availability**

529 The standalone VFSM code is available at <https://github.com/MPP-LSM/MPP>. The  
 530 ELM-VFSM code will be made available with the public release of E3SM model in  
 531 April, 2018.

## 532 **7 Competing interests**

533 The authors declare that they have no conflict of interest.



534

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539 programs.

540



541 **9 Tables**

542 **Table 1 Bias, root mean square error (RMSE), and correlation (R<sup>2</sup>) between**

543 **simulated water table depth and Fan et al. (2013) data.**

	<b>Bias [m]</b>	<b>RMSE [m]</b>	<b>R<sup>2</sup></b>
For all grids in ELM simulation with default $f_{drain}$	-10.3	21.3	0.28
For all grids in ELM simulation with optimal $f_{drain}$	2.10	8.33	0.91
For 79% grids with optimal $f_{drain}$ in ELM simulation with optimal $f_{drain}$	-0.04	0.67	0.99
For 21% grids without optimal $f_{drain}$ in ELM simulation with optimal $f_{drain}$	-9.82	18.08	0.31

544

545



546 **Table 2 ILAMB benchmark scores for latent heat flux (LH), sensible heat flux**  
 547 **(SH), total water storage anomaly (TWSA), and surface runoff. The calculation**  
 548 **of ILAMB metrics and scores are described at <http://redwood.ess.uci.edu/>.**

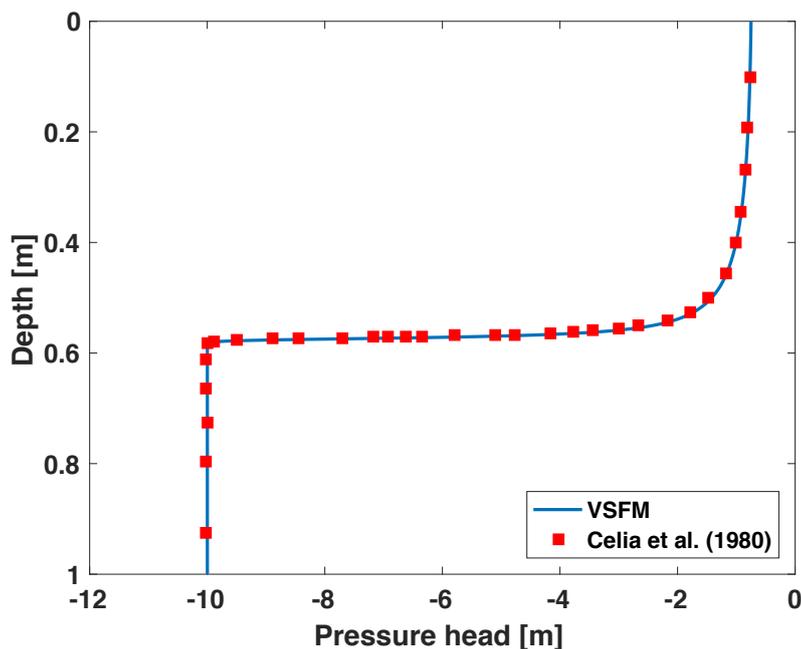
	Data Source	Simulation with default $f_d$			Simulation with optimal $f_d$		
		Bias	RMSE	ILAMB Score	Bias	RMSE	ILAMB Score
LH	FLUXNET	10.1 [Wm <sup>-2</sup> ]	21.0 [Wm <sup>-2</sup> ]	0.68	9.5 [Wm <sup>-2</sup> ]	21.3 [Wm <sup>-2</sup> ]	0.68
	GBAF	7.1 [Wm <sup>-2</sup> ]	16.3 [Wm <sup>-2</sup> ]	0.81	6.3 [Wm <sup>-2</sup> ]	16.3 [Wm <sup>-2</sup> ]	0.81
SH	FLUXNET	6.7 [Wm <sup>-2</sup> ]	22.5 [Wm <sup>-2</sup> ]	0.66	7.1 [Wm <sup>-2</sup> ]	22.8 [Wm <sup>-2</sup> ]	0.65
	GBAF	6.9 [Wm <sup>-2</sup> ]	21.2 [Wm <sup>-2</sup> ]	0.71	7.6 [Wm <sup>-2</sup> ]	21.7 [Wm <sup>-2</sup> ]	0.70
TWSA	GRACE	1.3 [cm]	7.8 [cm]	0.48	3.0 [cm]	9.6 [cm]	0.48
Runoff	Dai	-0.26 [kg m <sup>-2</sup> d <sup>-1</sup> ]	0.91 [m <sup>-2</sup> m <sup>-2</sup> d <sup>-1</sup> ]	0.52	-0.23 [kg m <sup>-2</sup> d <sup>-1</sup> ]	0.88 [kg m <sup>-2</sup> d <sup>-1</sup> ]	0.50

549

550

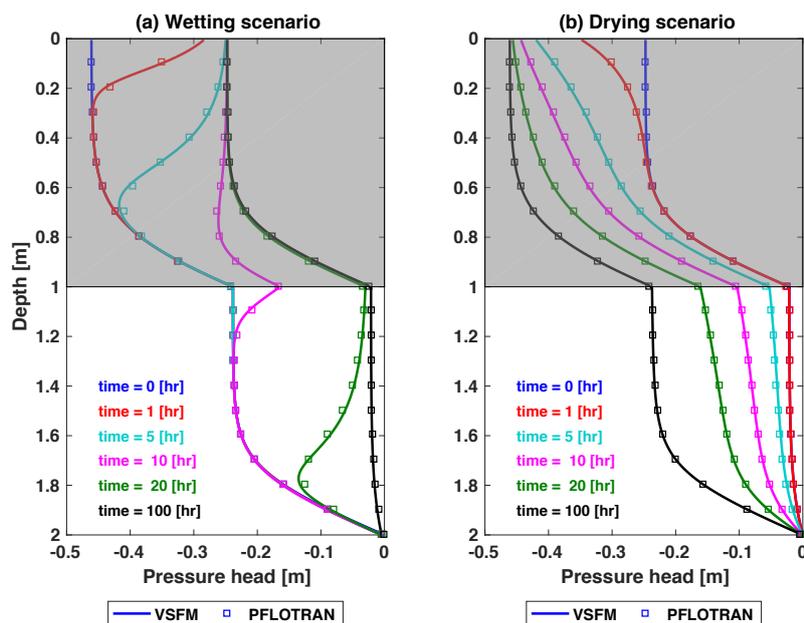


551 **10 Figures**



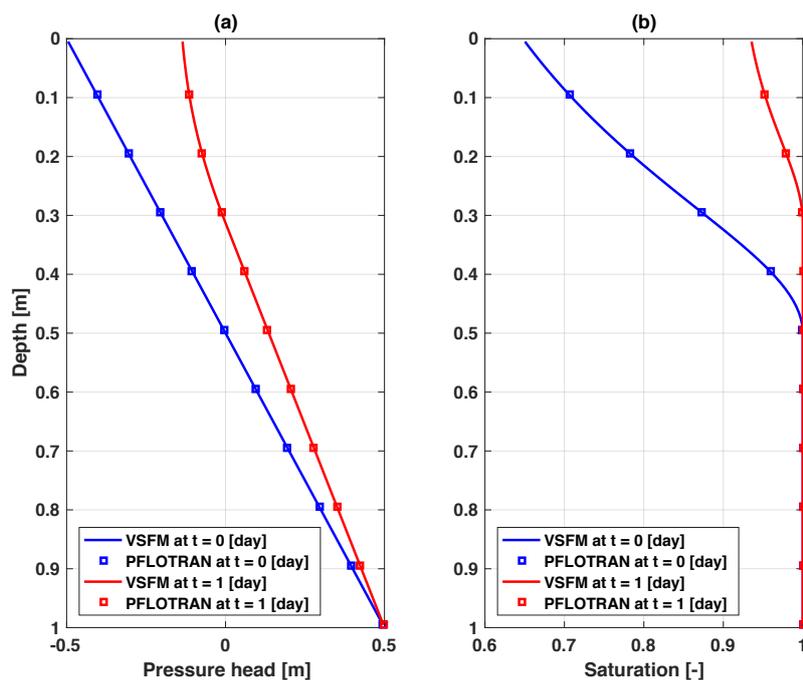
552

553 **Figure 1. Comparison of VSFM simulated pressure profile (blue line) against**  
554 **data (red square) reported in Celia et al. (1990) at time = 24 hr for infiltration**  
555 **in a dry soil column. Initial pressure condition is shown by green line.**



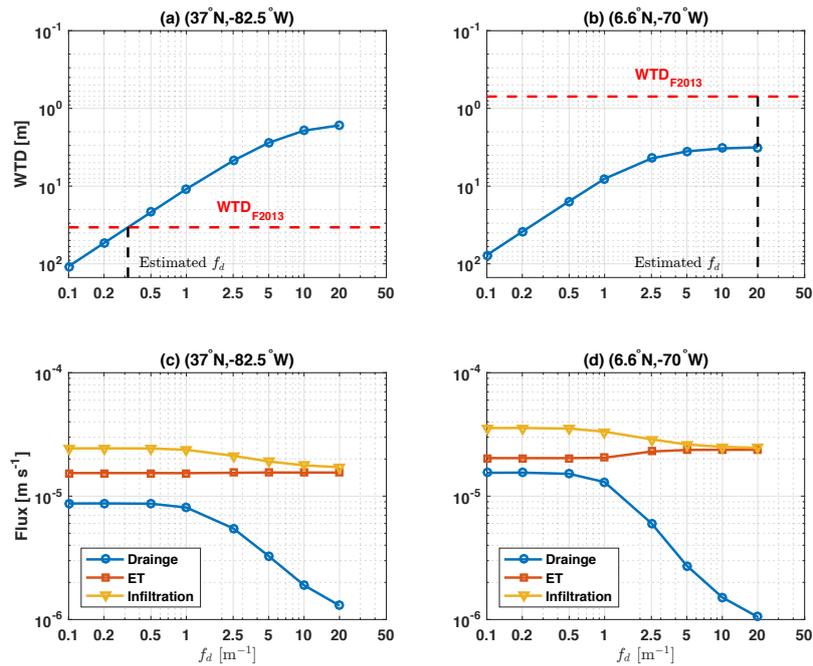
556

557 **Figure 2. Transient liquid pressure simulated for a two layer soil system by**  
558 **VSFM (solid line) and PFLOTRAN (square) for wetting (left) and drying (right)**  
559 **scenarios.**



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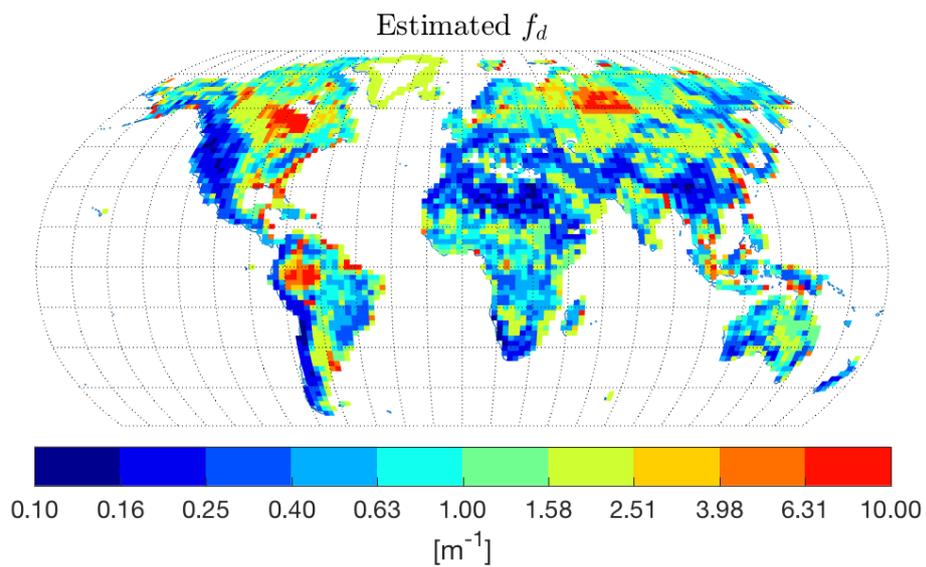
561 **Figure 3. Transient liquid pressure (a) and soil saturation (b) simulated by**  
562 **VSFM (solid line) and PFLOTRAN (square) for the water table dynamics test**  
563 **problem.**



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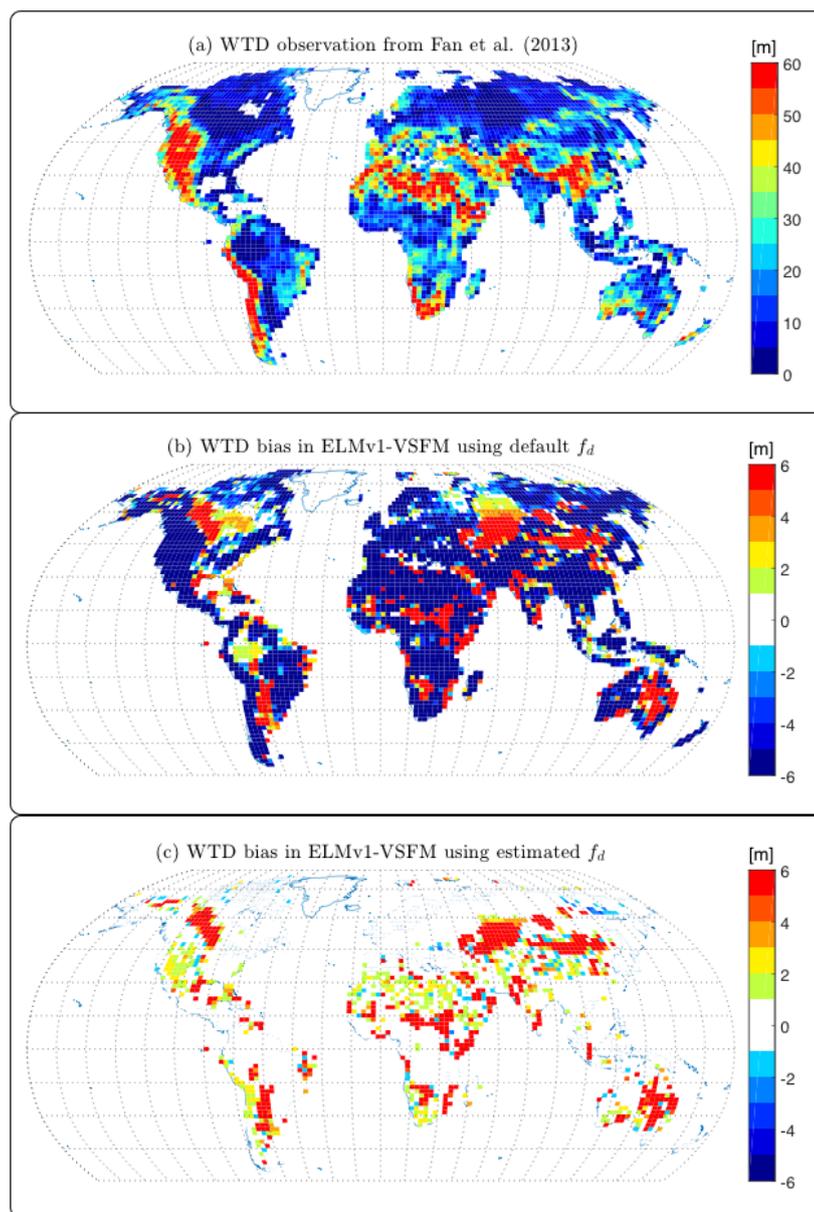
565 **Figure 4. (a-b) The nonlinear relationship between simulated water table**  
 566 **depth (WTD) and  $f_d$  for two gridcells within ELM's global grid. WTD from the**  
 567 **Fan et al. (2013) dataset and optimal  $f_d$  for the two gridcells are shown with a**  
 568 **dashed red and dashed black lines, respectively. (c-d) The simulated drainage,**  
 569 **evapotranspiration, and infiltration fluxes as functions of optimal  $f_d$  for the**  
 570 **two ELM gridcells.**

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572

573 **Figure 5. Global estimate of  $f_d$ .**

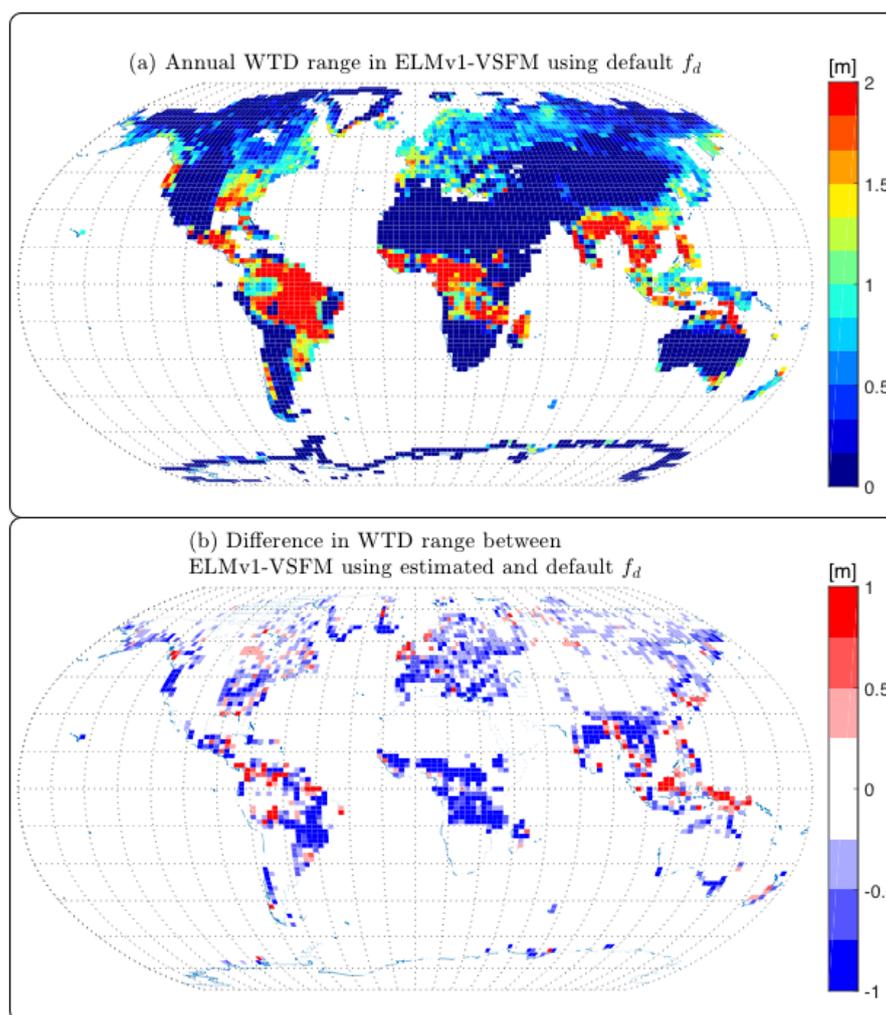


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575 **Figure 6. (a) Water table depth observation from Fan et al. (2013); (b) Water**  
576 **table depth biases (=Model - Obs) from ELMv1-VSFM using default spatially**  
577 **homogeneous  $f_d$ ; and (c) Water table depth biases from ELMv1-VSFM using**  
578 **spatially heterogeneous  $f_d$ .**



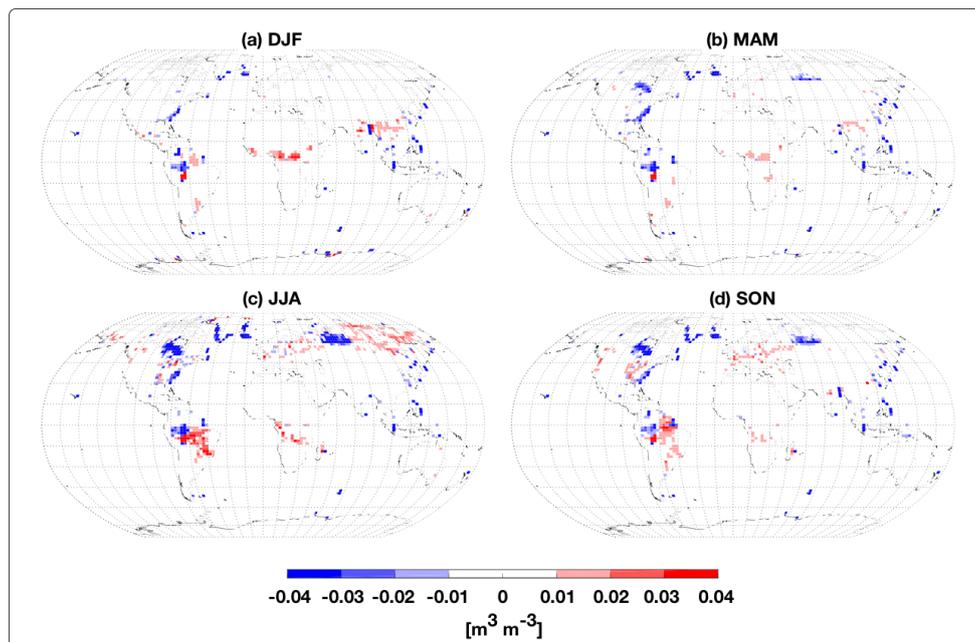
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581 **Figure 7. (a) Annual range of water table depth for ELMv1-VSFM simulation**  
582 **with spatially heterogeneous estimates of  $f_d$  and (b) Difference in annual**  
583 **water table depth range between simulations with optimal and default  $f_d$ .**

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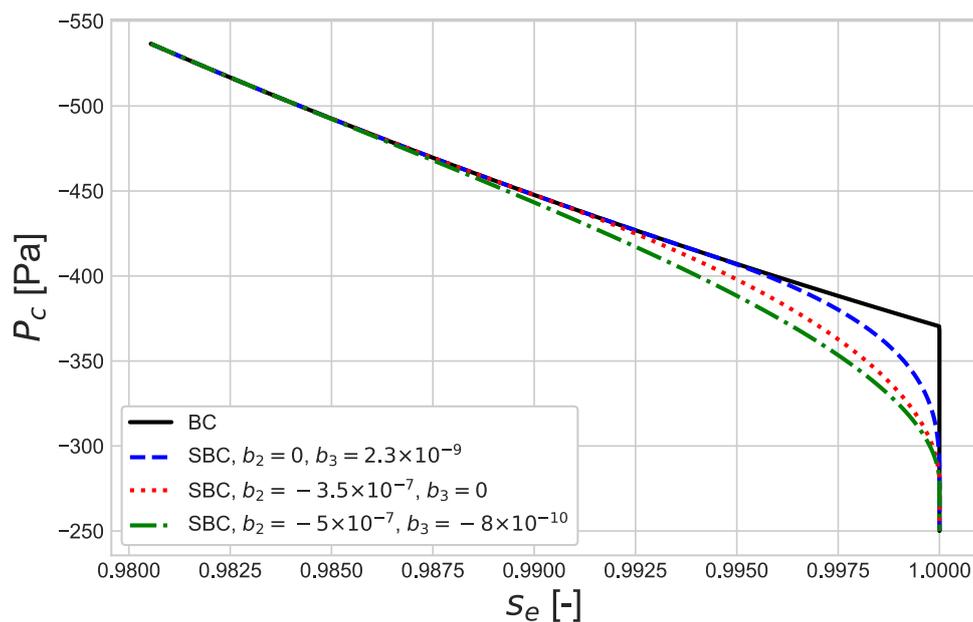
586 **Figure 8. Seasonal monthly mean soil moisture differences for top 10 cm**

587 **between ELMv1-VSFM simulations with optimal and default  $f_d$  values.**

588



589



590

591 **Figure A 1** The Brooks-Corey water retention curve for estimating liquid saturation,  $s_e$ ,

592 as a function of capillary pressure,  $P_c$ , shown in solid black line and smooth

593 approximation of Brooks-Corey (SBC) are shown in dashed line.

594

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