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Estimating macropore parameters for HYDRUS using a meta-model

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Abstract

The vertical change in the number of macropores causes a variation of the relative macroporosity (w_f) and the effective aggregate width (d_{ag}) over the soil profile. Both parameters are used in HYDRUS to represent this variation, increasing the number of parameters and making automated calibration challenging. The working hypothesis is that we can improve an analytical estimation of w_f and d_{ag} developed in previous research by inverse estimation with a meta-model for HYDRUS 2D/3D, using disk infiltrometer data of infiltration at zero pressure head. We generate a meta-model that describes the vertical heterogeneity of the macropore number with a general function using four parameters: the relative macroporosity at the soil surface (w_{fs}), the effective macropore radius (r_m), the maximum depth of macropores (z_{max}) and the shape parameter of the w_f curve (m). The meta-model computes the variation of w_f and d_{ag} over depth, thus reducing the parameters for automated calibration with HYDRUS. We theoretically described how to directly obtain the meta-model parameters with disk infiltrometer data, providing an example for field conditions. A complete parametrization of matrix and macropore parameters for HYDRUS 2D/3D was generated from these data and previous studies, which were updated by automated calibration. Only w_{fs} was calibrated, increasing by about ~3.5 times the initial measurement. We tied several macropore parameters to w_{fs} during calibration by their physical or mathematical relations. This methodology can be utilized to estimate HYDRUS parameters for risk assessment or detailed plot studies.

Highlights

- A meta-model to estimate macropore parameters for HYDRUS 2D/3D is presented.
- The meta-model reduces the number of macropore parameters for HYDRUS 2D/3D.
- Initial estimations of meta-model parameters are obtained by disk infiltrometer.

1 | INTRODUCTION

The heterogeneous distribution of the macroporosity and the geometry of the macropore network are characterized by unevenly distributed macropores over the soil profile, which results in the number of macropores changing over depth. In Urbina et al. (2019), this situation is mentioned as "heterogeneous macropore geometries." The uneven distribution of macropore numbers over depth was observed in Schon, Mackay, Gray, van Koten, and Dodd (2017) and is probably a common occurrence under field conditions. Simulation of heterogeneous macropore geometries under controlled conditions was performed by Urbina et al. (2019) for HYDRUS-1D (Šimůnek, van Genuchten, & Šejna, 2016) and SWAP (Kroes et al., 2017) computer codes. They found that the variation over depth of the relative macroporosity, w_f, and the effective aggregate width, d_{ag}, are critical parameters for simulating this uneven distribution in both models. Hence, advances in the estimation of w_f and d_{ag} for field conditions are essential for increasing the accuracy of dual-permeability model simulations.

A method of estimating w_f and d_{ag} under field conditions from disk infiltrometer data was developed by Urbina, van Dam, van den Berg, Ritsema, and Tang (2020). The resulting methodology allows an initial estimation of w_f and d_{ag} for dual-permeability models such as HYDRUS, SWAP and MACRO (Jarvis & Larsbo, 2012), including different macropore-matrix geometries. The methodology is based on quasi-steady-state one-dimensional water flow conditions. However, steady-state conditions are challenging to achieve for field environments (Šimůnek, Wendroth, & van Genuchten, 1999), and disk infiltrometer infiltration is commonly 3D instead of one-dimensional (Stewart et al., 2016; Alberti & Cey, 2011). Therefore, improvements in Urbina et al.'s (2020) methodology are necessary to adjust w_f and d_{ag} estimation for field conditions. The improvement can be performed by calibration using disk infiltrometer data as observations and a 3D dual-permeability model for simulations. This improvement is the primary goal of this research.

Measurements with a disk infiltrometer at zero pressure head allow accounting for infiltration into the macropore and matrix domains simultaneously. The infiltration in both domains can be simulated by HYDRUS 2D/3D, which incorporates axisymmetric flow around the vertical axis and a dual-permeability transfer model (Gerke & van Genuchten, 1993). The simulated data from HYDRUS 2D/3D can be used to update w_f, d_{ag} and other macropore parameters by calibration. Prior research applied manual calibration to obtain macropore parameters for HYDRUS 2D/3D using Guelph parameters and disk infiltrometers (Alberti & Cey, 2011; Kodesova, Simunek, Nikodem, & Jirku, 2010). However, fully automated calibration is a better alternative than manual calibration to accurately obtain fitted macropore parameters and uncertainty bounds.

The automated calibration of HYDRUS 2D/3D is challenging because the dual-permeability conceptualization in the model produces more numerical instabilities than the uniform flow conceptualization. Therefore, the ability to find reasonable initial estimates for macropore parameters is critical before calibration, along with reducing model complexity (Arora, Mohanty, & McGuire, 2011). Additionally, the parameters related to water and solute exchange between the macropore and matrix (Gerke & van Genuchten, 1996) vary concerning the density (number) of macropores (Arora et al., 2011; Urbina et al., 2019). Therefore, the number of macropore parameters (w_f and d_{ag}) increases considerably when the number of macropores varies over depth. This situation produces a challenging scenario for the automated calibration of HYDRUS 2D/3D under field conditions because it should be necessary to determine those parameters (w_f and d_{ag}) for each soil layer in the model. A meta-model for HYDRUS 2D/3D can overcome those drawbacks. Meta-models or surrogate models are defined in Asher, Croke, Jakeman, and Peeters (2015) as computationally cheaper models designed to approximate the dominant features of a complex model, which facilitates calibration and uncertainty analysis. An example of meta-modelling is found in Hack-ten Broeke et al. (2016), using the hydrological models SWAP-WOFOST. Ideally, the meta-model parameters should be easy to measure for field conditions and smaller in number than the original model.

We develop a meta-model in the R programming language for reducing the number of macropore parameters

(w_f and d_ag) in heterogeneous macropore geometries for HYDRUS 2D/3D. The meta-model solves the drawback of the increasing number of parameters in vertical heterogeneity of the macroporosity by a general function. An initial estimation of meta-model parameters with a disk infiltrometer is incorporated, which is next improved by calibration. The working hypothesis is that we can improve the analytical estimation of the relative macroporosity (w_f) and the effective aggregate width (d_ag) developed in Urbina et al. (2020) by inverse estimation with a meta-model for HYDRUS 2D/3D, using disk infiltrometer data of infiltration at zero pressure head. The objectives of this study are as follows: (a) conceptualize a meta-model to reduce the number of dual-permeability parameters during inverse estimation; (b) propose a methodology for an independent measurement of meta-model parameters with disk infiltrometer data; and (c) provide an example of applying the meta-model under field conditions with disk infiltrometer data using HYDRUS 2D/3D for simulations. We refer to HYDRUS-1D/2D/3D collectively as HYDRUS, except when explicitly referring to the dimensionality of the model (e.g., HYDRUS-1D) is necessary.

2 | MATERIALS AND METHODS

2.1 | HYDRUS model

The HYDRUS code uses the dual-permeability model presented in Gerke and van Genuchten (1993). This model solves two Richards equations, one for the matrix domain and the other for the macropore (fracture) domain, and couples them by a water exchange term:

$$C_f \frac{\partial h_f}{\partial t} = \frac{\partial}{\partial z}\left(K_f \frac{\partial h_f}{\partial z} - K_f\right) - \frac{\Gamma_w}{w_f}, \tag{1a}$$

$$C_m \frac{\partial h_m}{\partial t} = \frac{\partial}{\partial z}\left(K_m \frac{\partial h_m}{\partial z} - K_m\right) + \frac{\Gamma_w}{1 - w_f}, \tag{1b}$$

where C is the specific water capacity ($\frac{\partial \theta}{\partial h}$) cm^{-1}, h is the pressure head (cm), K is hydraulic conductivity (cm min^{-1}), z is depth (cm) and t is time (min). The subscripts f and m refer to fracture or matrix, respectively. Γ_w is the water transfer term (min^{-1}) computed as:

$$\Gamma_w = \alpha_w \left(h_f - h_m\right), \tag{2a}$$

$$\alpha_w = \frac{\beta}{d_{ag}^2} \gamma_w K_a(h), \tag{2b}$$

where β is a dimensionless geometry-dependent coefficient, d_ag is the effective aggregate width (cm), which represents an effective distance between the wall of the macropores and the centre of the matrix, γ_w is a dimensionless scaling coefficient (usually taken as 0.4) and K_a (h) is the effective hydraulic conductivity evaluated in terms of both h_f and h_m. β can be obtained from d_ag and the macropore radius (r_m, cm) for cylindrical macropores surrounded by a cylindrical matrix mantle (Gerke & van Genuchten, 1996):

$$\beta = \frac{1}{[0.19\ln(16\zeta_0)]^2}; where \ \ 1 < \zeta_0 < 100 \, and \, \zeta_0 = \frac{d_{ag} + r_m}{r_m}. \tag{3}$$

The dual-permeability model of Gerke and van Genuchten (1993) was incorporated in HYDRUS 2D/3D, keeping the same conceptualization and parameters mentioned above for the 1D case.

We defined "macropore layers" according to the variation of the macropore numbers in the soil profile, which produce variation in the lateral transfer parameters (w_f, d_ag, and β) in HYDRUS. Therefore, "macropore layers" is a concept concerning HYDRUS and not related to pedology. Those macropore layers may be in one homogeneous soil matrix horizon described for field conditions. For example, in Figure 1 (III), eleven macropore layers and three matrix layers (or soil horizons) are present. The macropore layers are generated at each macropore ending.

Twenty-two values of w_f and d_ag are required in HYDRUS to represent the problem in Figure 1 ($w_\mathrm{f,j}$, and $d_\mathrm{ag,j}$, where $j = 1,2,...,11$). β is not counted because it is mathematically related to d_ag (Equation (3)). The meta-model replaces these twenty-two values with four parameters (next section), which reduces the complexity of modelling heterogeneous macropore geometries. Hence, the meta-model enables HYDRUS to be independent of the number of macropore layers or independent of the effect that produces the vertical variation of the macropore number on lateral transfer parameters (w_f, $d_\mathrm{ag,}$ and β).

One strong assumption in the dual permeability conceptualization of HYDRUS is that the macropore connects the top and bottom boundaries. Therefore, it is not possible to include explicitly dead-end pores. However, dead-end pores are related to an increase in the lateral exchange of water. Thus, they can be implicitly represented by the computation of d_ag regarding the vertical distribution of the macropore number. This option was used in Urbina et al. (2019) to represent implicitly dead-end pores in controlled laboratory conditions with HYDRUS-1D.
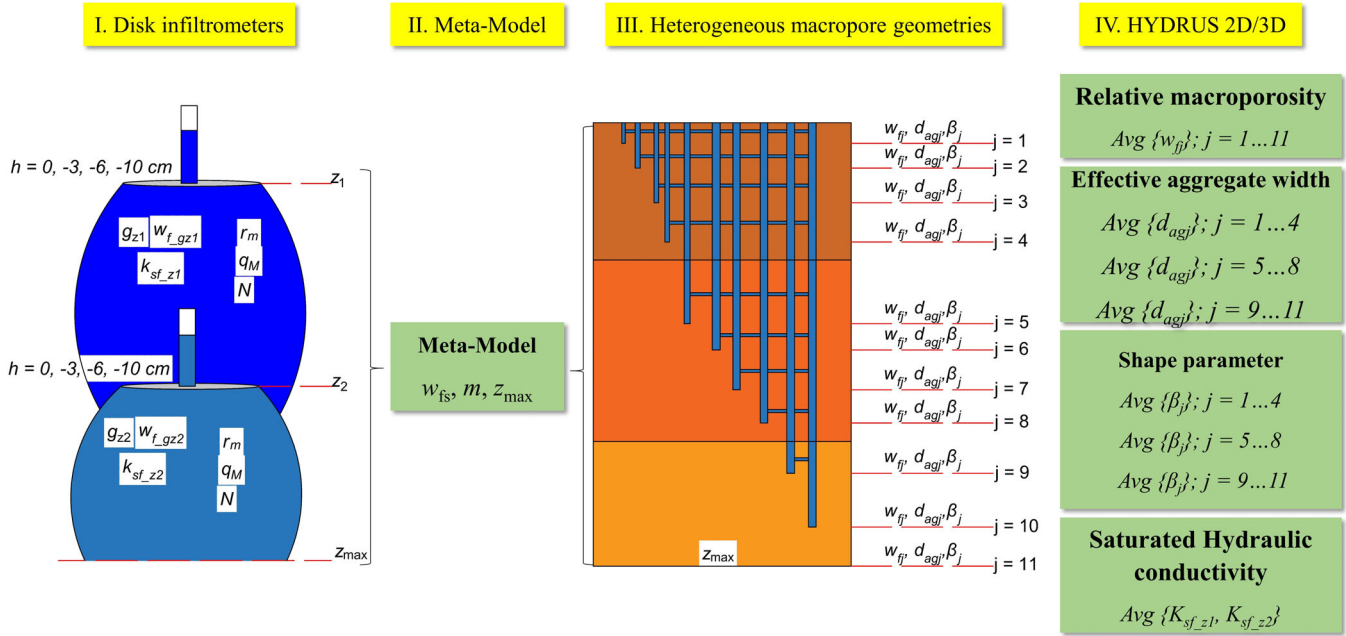
FIGURE 1 The schematization for initial measurements of HYDRUS 2D/3D macropore parameters by a meta-model. Part I depicts the variables obtained from disk infiltrometer measurements at two depths, z_1 and z_2. Part II shows the generation of meta-model parameters from the variables obtained in Part I. Part III illustrates the use of the meta-model under heterogeneous macropore geometries for generating the relative macroporosity w_{fj}, the effective aggregate width d_{agj} and the shape parameter β_j for each macropore layer j. Part IV demonstrates how the different parameters are averaged (Avg) in HYDRUS 2D/3D [Color figure can be viewed at wileyonlinelibrary.com]

2.2 | Meta-model

The meta-model for HYDRUS is based on a continuous decrease of the relative macroporosity (w_f) over the soil profile:

$$w_{f\_z} = w_{fs} * \left(1 - \frac{z}{z_{max}}\right)^m, \qquad (4)$$

where w_{f_z} (cm^3 cm^{-3}) is the relative macroporosity at depth z (cm), w_{fs} (cm^3 cm^{-3}) is the relative macroporosity at the soil surface (maximum w_f), z is the vertical coordinate (cm; positive upward, zero at the soil surface), z_{max} (cm) is the bottom of the active macropore layer (where $w_f = 0$) and m is a shape factor for the w_f curve.

The relative macroporosity (w_f) and the effective aggregate width (d_{ag}) are mathematically related (Urbina et al., 2020). For cylindrical macropores surrounded by a cylindrical matrix mantle d_{ag} is computed as follows (Urbina et al., 2019):

$$d_{ag} = r_m \left(\frac{1}{\sqrt{w_f}} - 1\right) \ where: w_f \ ]0,1]. \qquad (5)$$

The reduction of macropore parameters in HYDRUS with the meta-model is performed by computing w_f over depth by Equation (4) and then replacing those values in Equation (5) to obtain d_{ag} over depth. Researchers should note that w_f and d_{ag} can be obtained from Equations (4)

and (5) with a resolution as small as 1 cm; therefore, several macropore layers can be generated and set in the HYDRUS model. On the other hand, those parameters can be averaged to represent each soil matrix layer (or soil horizon) in HYDRUS (Figure 1 (IV)). The average for macropore parameters introduced in Figure 1 (IV) is generally optional, which means researchers can set in HYDRUS an arbitrary number of macropore layers. The only parameter that must be averaged over the soil profile for HYDRUS is the relative macroporosity (w_f), as is observed in the next sections.

The meta-model is written in R script. The previous equations for the meta-model use input parameters different to those in HYDRUS; therefore, a pre-processing is included in the R script to obtain HYDRUS parameters. This pre-processing included the steps depicted in Figure 1 for averaging the parameters. After the pre-processing, the R script runs HYDRUS internally.

The meta-model parameters can be independently estimated under field conditions because they have either physical (w_{fs}, z_{max}, and r_m) or geometrical (m) meaning. In the next section, we propose disk infiltrometers to estimate the meta-model parameters for field conditions.

2.3 | Disk infiltrometers

The disk infiltrometer is a device that allows for the measurement of infiltration rates at different pressure heads

imposed at the base of a disk (Perroux & White, 1988). These pressure heads can be transformed into a macropore radius (Equation (6)) using the Young-Laplace capillarity theory. For water at 20°C and a contact angle of zero between the liquid–vapour–solid interface, the equivalent macropore radius (r_m) for a given pressure head (h) is:

$$r_m \cong \frac{-0.15}{h} \, cm, \tag{6}$$

where h (cm) is the pressure head imposed at the base of the disk infiltrometer.

Let us assume throughout the next sections that a disk infiltrometer is employed at {0, −3, −6 and −10} cm pressure head. We can generate pressure head ranges such as (0, −3), (−3, −6) and (−6, −10) cm, where the macropore water flux is measured at steady-state flow conditions. The minimum radius of each pressure head range is 0.05, 0.025 and 0.015 cm (Equation (6)), respectively. We considered a value of −10 cm for the threshold pressure head between the macropore and matrix domains (Jarvis et al., 2007).

The steady-state flux rates (q_M, cm min^{-1}) are computed as follows:

$$q_{M\_0} = q_{M[0,-3]} + q_{M[-3,-6]} + q_{M[-6,-10]} + q_{M[matrix]}, \tag{7}$$

where q_{M_0} is the steady-state flux rate measured at zero pressure head and $q_{M[0,-3]}$ is the steady-state flux rate obtained by subtracting q_{M_3} from q_{M_0}. A similar computation is performed for $q_{M[-3,-6]}$ and $q_{M[-6,-10]}$. Dividing Equation (7) by q_{M_0} yields the flux proportion associated with each macropore size range.

The number of cylindrical macropores per unit area, N (m^{-2}), is obtained by applying the Hagen-Poiseuille equation and Darcy's law, assuming laminar flow conditions (Dunn & Phillips, 1991; Watson & Luxmoore, 1986):

$$N = \frac{q_M \, 8 \eta}{\pi \rho \, g \, r_m^4}, \tag{8}$$

where η (Kg m^{-1} s^{-1}) is the dynamic viscosity of water, ρ (kg m^{-3}) is the density of water and g (m s^{-2}) is the gravitational constant. Equation (8) is computed for different pressure heads because of q_M and r_m (Equation (6)). The total number of macropores, N_T (m^{-2}), is obtained by:

$$N_T = N_{[0,-3]} + N_{[-3,-6]} + N_{[-6,-10]}, \tag{9}$$

where $N_{[0,-3]}$ is the number of macropores per unit area using $q_{M\,[0,-3]}$ and $r_m = 0.05$ cm in Equation (5). A similar computation is performed for $N_{[-3,-6]}$ and $N_{[-6,-10]}$.

The relative macroporosity, w_f, can be computed using disk infiltrometer data as follows:

$$w_f = N * A_m, \tag{10}$$

where A_m is the average macropore cross-sectional area (m^2). Both N and A_m in Equation (10) are computed for different pressure heads. Hence, the final relative macroporosity is obtained as follows:

$$w_f = w_{f[0,-3]} + w_{f[-3,-6]} + w_{f[-6,-10]}, \tag{11}$$

where $w_{f(0,-3)}$ is computed using $N_{[0,-3]}$ and $r_m = 0.05$ cm in Equation (10), and similarly for $w_{f[-3,-6]}$ and $w_{f[-6,-10]}$.

2.4 | Computation of meta-model parameters with disk infiltrometers

In previous sections, we indicated how to compute the relative macroporosity with disk infiltrometers, including different pressure head ranges. These concepts are relevant for obtaining initial estimations of meta-model parameters (Equations (4) and (5)). Equation (4) computes the relative macroporosity at depth z in the soil profile. Therefore, to obtain Equation (4) parameters, we need to place the disk infiltrometer in at least two depths, z_1 and z_2, for different pressure heads (Figure 1 (I)). Researchers should note that by placing the disk infiltrometer at depths z_1 and z_2, an average relative macroporosity is obtained. For example, when placing the disk infiltrometer at the soil surface ($z_1 = 0$), the measurement of the relative macroporosity by Equation (11) represents an average from z_1 until a depth z (unknown) (Figure 1_I). The average relative macroporosity and its depth are denoted by the letter "g" in Equations (12) to (15). From previous infiltration rate measurements with the disk infiltrometer at two depths, the relative macroporosity at the soil surface, w_{fs}, and the shape factor parameter, m (see Equation (4)), are obtained as follows:

$$w_{f\_g_{z1}} = w_{fs} * \left(1 - \frac{g_{z1}}{z_{max}}\right)^m ; depth \, z_1, \tag{12}$$

$$w_{f\_g_{z2}} = w_{fs} * \left(1 - \frac{g_{z2}}{z_{max}}\right)^m ; depth \, z_2. \tag{13}$$

Combining Equations (12) and (13) obtains:

$$w_{fs} = w_{f\_g_{z1}} \left(1 - \frac{g_{z1}}{z_{max}}\right)^{-m}, \qquad (14)$$

$$m = \ln\left(\frac{w_{f\_g_{z2}}}{w_{f\_g_{z1}}}\right) \left[\ln\left(\frac{z_{max} - g_{z2}}{z_{max} - g_{z1}}\right)\right]^{-1}, \qquad (15)$$

where $w_{f\_g_{zx}}$ represents an average relative macroporosity located at depth g_{zx} (cm) (Equations (12) and (13)). $w_{f\_g_{zx}}$ is computed by Equation (11); therefore, Equations (14) to Equation (15) can be applied individually to different pressure head ranges.

Equations (14) and (15) allow the estimation of w_{fs} and m in Equation (4). The depths g_{z1}, g_{z2} and z_{max} (Equations (12) to (15)) are initially subjectively chosen and are set constant over the different pressure head measurements. However, we anticipate that the depths g_{z1} and g_{z2} are updated during calibration.

The parameter d_{ag} can now be computed for different depths and pressure head ranges using Equation (5). However, d_{ag} cannot be set for different pressure head ranges in the HYDRUS model. Therefore, the computation of an average effective aggregate width, $\bar{d}_{ag}$ (cm), using different pressure head ranges is necessary for obtaining a singular value. This $\bar{d}_{ag}$ is computed at every macropore layer over depth (Figure 1 (III)). The $\bar{d}_{ag}$ is obtained from the disk infiltrometer measurements as follows:

$$\overline{d_{ag}} = d_{ag[0,-3]} * \frac{q_{M[0,-3]}}{q_{M\_0}} + d_{ag[-3,-6]} * \frac{q_{M[-3,-6]}}{q_{M\_0}}$$
$$+ d_{ag[-6,-10]} * \frac{q_{M[-6,-10]}}{q_{M\_0}}, \qquad (16)$$

$d_{ag(0,-3)}$ is computed with Equation (5) where $r_m = 0.05$ cm and $w_f = w_{f(0,-3)}$. The same holds for $d_{ag(-3,-6)}$ and $d_{ag(-6,-10)}$ cm. Equation (16) shows that the average $\bar{d}_{ag}$ is weighted by water flow.

2.5 | Saturated hydraulic conductivity of macropores

The meta-model is not related to the computation of the saturated hydraulic conductivity of the macropores (K_{sf}, cm min^{-1}), although K_{sf} is required for the dual-permeability model of HYDRUS. The initial estimation of K_{sf} based on cylindrical macropores can be performed by combining the Hagen-Poiseuille equation and Darcy's law for laminar flow conditions (Dunn & Phillips, 1991; Watson & Luxmoore, 1986):

$$K_{sf} = \frac{\rho * g}{8 * \eta} \left(r_{m\_3}{}^2 * \frac{N_{[0,-3]}}{N_T} + r_{m\_6}{}^2 * \frac{N_{[-3,-6]}}{N_T} + r_{m\_10}{}^2 * \frac{N_{(-6,-10)}}{N_T}\right), \qquad (17)$$

where r_{m_3} (cm) is the maximum macropore radius computed for pressure head −3 cm (Equation (6)), with similar consideration for r_{m_6} and r_{m_10}. The total number of macropores, N_T, is computed with Equation (9). Equation (17) for K_{sf} is based on the arithmetic mean of parallel stratified media (Jang, Narsilio, & Santamarina, 2011), weighted by the number of macropores for each pressure head range (e.g., $N_{(0,-3)}$ to N_T). The K_{sf} solution in Equation (17) is valid for horizontal, vertical and sloped macropore directions.

The previous methodology allows us to directly estimate w_{fs}, m, d_{ag} and K_{sf} by disk infiltrometer measurements, whereas g_{z1}, g_{z2} and z_{max} are initially subjectively chosen. One way to estimate all these parameters directly without subjective suppositions is by placing the disk infiltrometer within at least five depths (five unknowns in Equations (12) to (15)). However, that procedure is out of the scope of this research.

2.6 | Field example

A field site with Spruce trees was selected to test the meta-model developed in previous sections. The field site is in Valkenburg, the Netherlands (N50°51.515/ E005°53.684, elevation 117 m). The 20-year average precipitation and average temperature until 2019 are 763.3 mm and 10.84°C, whereas the 10-year average precipitation and average temperature until 2019 are 726.4 mm and 10.85°C. The field site was not ploughed for 8 years. Therefore, a significant macropore presence was expected. Only cylindrical macropores were observed in the field. The textural class changed from clay loam at the topsoil to clay at the subsoil. The soil was found to be hydrophilic at the top 50 cm; below that, no measurements were performed.

Undisturbed soil core samples of 8 cm high and 10 cm in diameter were taken at the soil surface, and at 18.5 and 33-cm depth, after the disk infiltrometer measurement. The measurements were obtained directly below the place where the disk infiltrometer was set. The samples' depths were selected to represent each soil horizon present to a depth of 50 cm.

The undisturbed soil cores were analysed in the Soil Hydro Physics Laboratory of Wageningen University & Research Centre. The soil hydraulic matrix parameters were determined using the evaporation method. Four mini tensiometers were installed at 2-cm intervals, and at 1 cm from the top and bottom boundaries of the soil core.

The measured soil water pressure head and soil evaporation were analysed through calibration using HYDRUS-1D (Šimůnek, van Genuchten, & Wendroth, 1998), setting the residual water content (θ_r, cm^3 cm^{-3}) to the default value provided by HYDRUS-1D for clay. Next, the saturated water content (θ_s, cm^3 cm^{-3}), the inverse of the air entry value (α, cm^{-1}), the pore size distribution (n), the saturated hydraulic conductivity (K_s, cm min^{-1}) and the pore connectivity (l) parameters of the matrix were calibrated. Care was taken to ensure the same measured and simulated evaporation at the end of the optimization.

The derived van Genuchten-Mualem parameters (θ_r, θ_s, α, n, K_s, l) and the bulk density (D_a, g cm^{-3}) are presented in Table 1. The bulk density was obtained using the undisturbed soil cores at the end of the evaporation method (ISO 11272, 1993).

A tension disk infiltrometer of 20 cm diameter (Commonwealth Scientific and Industrial Research Organisation, Disk Permeameter) was set at $z_1 = 0$ and $z_2 = 30$ cm depth. For each measurement, around 1 cm of coarse sand was placed and levelled. At the soil surface, all grass was removed by cutting it as much as possible.

Infiltration rate measurements were performed at the soil surface (z_1) for 0, −3 and −6 cm pressure head until a steady-state was reached. The measurement at 0 cm pressure head was performed first. One hour later, measurements at −6 and −3 cm pressure head were performed. After that, a pit was gently dug directly below the position where the previous measurement was taken. The disk infiltrometer was placed in this new position (z_2), and the infiltration rate was measured only for 0 cm pressure head at steady-state conditions.

The infiltration rate measured at the soil surface for 0 cm pressure head was measured in short time intervals until steady-state because that information is used for calibration with HYDRUS 2D/3D. A total of 34 measurements were performed in 58 min with a disk infiltrometer.

The steady-state flow rates, q_{M_0}, $q_{M\,[0,-3]}$ and $q_{M\,[-3,-6]}$ in Equation (7), were directly obtained from measurements at depth $z_1 = 0$ cm. The steady-state flow rate, $q_{M\,[-6,-10]}$, was estimated for depth z_1 as follows:

$$q_{M[-6,-10]} = q_{M\_0} - q_{M[0,-3]} - q_{M[-3,-6]} - q_{M[matrix]}. \quad (18)$$

The steady-state flow rate for the matrix, $q_{M[matrix]}$, was estimated as follows (Moene & van Dam, 2013):

$$q_{M(matrix)} = \frac{\sum\limits_{k=1}^{N_h} L_{mk}}{\sum\limits_{k=1}^{N_h} \frac{L_{mk}}{K_{sk}}}, \quad (19)$$

where $N_h = 3$ is the number of matrix layers, L_{mk} (cm) is the thickness of each matrix layer k, and K_{sk} (cm min^{-1}) is the saturated hydraulic conductivity of the matrix layer k. We assumed that $q_{M[matrix]}$ is equal to the composite saturated hydraulic conductivity obtained by Equation (19) under steady-state conditions (Watson & Luxmoore, 1986). The number of matrix layers, L_{mk}, and the saturated hydraulic conductivity, K_{sk} of each matrix layer (k), are found in Table 1.

The measurement at depth $z_2 = 30$ cm was only performed for a steady-state flow rate at 0 cm pressure head, q_{M_0}. The ratio between q_{M_0} measured at depth z_2 and z_1 was 0.39 (Table 2). The ratio was multiplied with q_{M_3}, q_{M_6} and q_{M_10} (Equation (7)) measured and estimated at the soil surface to generate those values for z_2. Therefore, we assume the decrease of steady-state flow, q_{M_0} in z_2 relative to z_1, proportionally reduced q_{M_3}, q_{M_6} and q_{M_10}. A summary of the steady-state flow rate measurements is given in Table 2.

The meta-model parameters w_{fs} and m (Equation (12) to Equation (15), respectively) were computed by setting the depths $g_{z1} = -15$, $g_{z2} = -50$ and $z_{max} = -100$ cm. The values of $w_{f\_gz1} = 9.14 * 10^{-4}$ and $w_{f\_gz2} = 3.26 * 10^{-4}$ were computed using Equations (12) and (13) (See Supplementary Material). The outcomes were $w_{fs} = 1.25 * 10^{-3}$ and $m = 1.94$. The values of g_{z1} and g_{z2} were chosen to be close to the measurement depth of the disk infiltrometer (z_1 and z_2) because we expected many macropores close to the soil surface. The value of z_{max} means that we do not expect macropores below 100 cm depth.

The initial gravimetric soil water content was measured at 45 and 40 cm away from the outer disk infiltrometer ring, and both samples were merged into

TABLE 1 The van Genuchten-Mualem parameters (θ_r, θ_s, α, n, K_s, l) and the bulk density (D_a) for the three soil horizons described in the field site

Depth (cm)	θ_r	θ_s	α (cm^{-1})	n	K_s (cm min^{-1})	l	D_a (g cm^{-3})
0–10	0.0950	0.5018	0.0049	1.3521	0.0266	10.0577	1.4119
10–30	0.0950	0.4482	0.0180	1.2526	0.0049	0.5785	1.3937
30–50	0.0950	0.4462	0.0074	1.4535	0.0086	3.6620	1.5931

TABLE 2 The steady-state flux rate measured at 0 (q_{M_0}), −3 (q_{M_3}) and −6 (q_{M_6}) cm pressure head

Depth (cm)	m s^{-1}						
	q_{M_0}	q_{M_3}	q_{M_6}	$q_{M\,[matrix]}$	$q_{M\,[0,-3]}$	$q_{M\,[-3,-6]}$	$q_{M\,[-6,-10]}$
$z_1 = 0$	1.53E-04	2.33E-05	1.00E-05	1.41E-06	1.30E-04	1.33E-05	8.59E-06
$z_2 = 30$	6.00E-05	9.13E-06	3.91E-06	1.41E-06	5.09E-05	5.22E-06	2.51E-06

Note: The steady-state flux rates measured at pressure head range [0, _3], [_3, _6] cm and estimated at [_6, _10] cm by Equation (18) are denoted as $q_{M[0,\_3]}$, q_M $_{[-3,\_6]}$ and $q_{M[-6,\_10]}$, respectively. Measurements and estimations of steady-state flow rate were performed at soil depth z_1 and z_2.
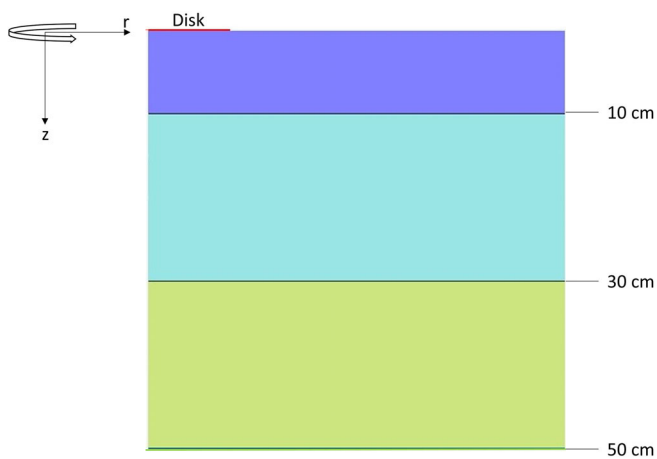

FIGURE 2 Schematic representation of HYDRUS 2D/3D using a square domain of 50 × 50 cm. In the top left corner, the radius of the disk infiltrometer is represented by a red line of 10 cm. At the bottom part of the domain, a free drainage bottom boundary condition is represented by a green line. The arrow indicates an axisymmetric flow about the vertical axis. Three soil horizons with their corresponding depths at 10, 30 and 50 cm are depicted [Color figure can be viewed at wileyonlinelibrary.com]

one sample. The initial water content was measured at every 10 cm up to a maximum depth of 80 cm. The samples were weighed on-site on a small scale and then oven-dried at 105°C. The initial gravimetric soil water content was transformed into volumetric water content with the bulk density of the soil (Figure S2, Supplementary Material).

2.7 | HYDRUS 2D/3D set up

The axisymmetric flow around the vertical axis was set in HYDRUS 2D/3D to simulate disk infiltrometer infiltration. The disk infiltrometer radius was represented by a red line of 10 cm at the top left corner (Figure 2). A square domain of 50 × 50 cm was set in HYDRUS 2D/3D, and three matrix and macropore layers were included in the model (Figure 2). The matrix and macropore layers corresponded to the soil horizons observed under field conditions. The dual-permeability

module of HYDRUS 2D/3D was applied for the simulations.

The time and space discretization for HYDRUS 2D/3D were set to obtain a mass balance error lower than 0.5% at every time step. The initial soil water content was set as a pressure head, transforming the initial volumetric water content (Figure S2, Supplementary Material) using the soil hydraulic matrix parameters (Table 1). The boundary condition for the disk infiltrometer (red line in Figure 2) was set as a constant head equal to zero. The bottom boundary condition was set as free drainage. All other boundaries were set as no flux boundaries. The model was run for 58 min, which corresponds to the disk infiltrometer measurement at zero pressure head in the soil surface.

The previous estimations of meta-model parameters (w_{fs}, m and z_{max}), along with Table 2, are sufficient to generate initial estimations of w_f, d_{ag} and K_{sf} in HYDRUS 2D/3D. Researchers should notice that the meta-model was generated at centimetre-scale until $z_{max} = 100$ cm (see Table S1, Supplementary Material). The simulation with HYDRUS 2D/3D terminates at 50-cm depth simply because, in this example, we did not measure the soil matrix at deeper layers.

The relative macroporosity cannot vary over depth in the HYDRUS 2D/3D version 2. xx. Therefore, an average value over depth should be computed before incorporating that parameter into the model (see Urbina et al., 2019). This issue is depicted in Figure 1 (IV), where the 11 w_{fj} are averaged to generate the input parameter for HYDRUS 2D/3D. It was decided to average d_{ag} and β to generate a unique value for each soil matrix layer (Figure 1 (IV)). Two values of K_{sf} were obtained, applying Equation (14) from disk infiltrometer measurements at z_1 and z_2 (Figure 1 (I)). In this research, the average of K_{sf} at the two depths is computed and set constant over depth for HYDRUS 2D/3D (Figure 1 (IV)). However, this is optional because the HYDRUS code allows different K_{sf} over depth. The above-mentioned computations of w_{fs}, m, w_f, d_{ag}, β and K_{sf} (Table 3) are available in the Supplementary Material.

The remaining macropore parameters in Table 3 were estimated as follows. The van Genuchten macropore

parameters (subscript f) θ_{rf} and θ_{sf} were set to represent a macropore that dries completely and transport water almost using the whole pore volume. The parameters α_f and n_f were set like the ones for sandy soil. The pore connectivity parameter of macropores l_f and the empirical factor γ ($-$) were fixed to 0.5 and 0.4, respectively. The effective hydraulic conductivity of the fracture-matrix interface, K_a (cm min^{-1}), was set equal to the saturated hydraulic conductivity of the matrix, K_s (Table 1).

2.8 | Calibration strategy

The model-independent Parameter Estimation δ Uncertainty Analysis (PEST) package (Doherty, 2015) was used for the calibration of the initially estimated meta-model and HYDRUS 2D/3D parameters (Table 3). The strategy was to calibrate the meta-model parameters running the R script with PEST. Therefore, PEST reads the input and output files generated by the R script for the meta-model, which runs HYDRUS 2D/3D internally after pre- and post-processing. This calibration was made possible by transforming the R script into a Batch file for Windows.

The meta-model parameter selected for calibration was the relative macroporosity at the soil surface, w_{fs}, because it can generate other model parameters via the analytical equations presented in the previous sections. Therefore, the change in w_{fs} performed by PEST at each iteration produces a variation in other model parameters. This interaction between parameters during calibration is illustrated by a tree chart (Figure 3).

The red boxes (Figure 3) mean that those variables were fixed during calibration (e.g., $w_{fs[0,-3]}$). The reason for fixed $w_{fs[0,-3]}$ is related to an overestimation of the water flow by the physical assumptions in the methodology (e.g., Hagen-Poiseuille equation, see Urbina et al., 2020). The overestimation of water flow produces an underestimation of w_{fs} and an overestimation of K_{sf}. One way to increase the final value of w_{fs} and decrease the value of K_{fs} simultaneously is by fixing $w_{fs[0,-3]}$ during calibration.

PEST was operated in "estimation mode," which minimizes the objective function with the Gauss-Marquardt-Levenberg method. The observed data (cumulative infiltration at 0 cm pressure head in the soil surface) were compared against the simulated cumulative infiltration of HYDRUS 2D/3D at 0 cm pressure head (red line in Figure 2). The observed data were divided into three groups, which facilitates the calculation of the weights. The PEST module PWTADJ1 computed the weights of each observational data group. They have been calculated with the condition that all observation data groups had the same importance in the objective function (ϕ). Therefore, the three cumulative infiltration groups had the same importance after the residual was multiplied by the weight (Equation (20)):

$$\phi = \sum_{i}^{i=Nt} (w_i \, r_{ei})^2, \qquad (20)$$

where Nt is the total number of observations, w_i is the weight associated with the i'th observation, and r_{ei} (cm) is the i'th residual (difference between model output and measurement).
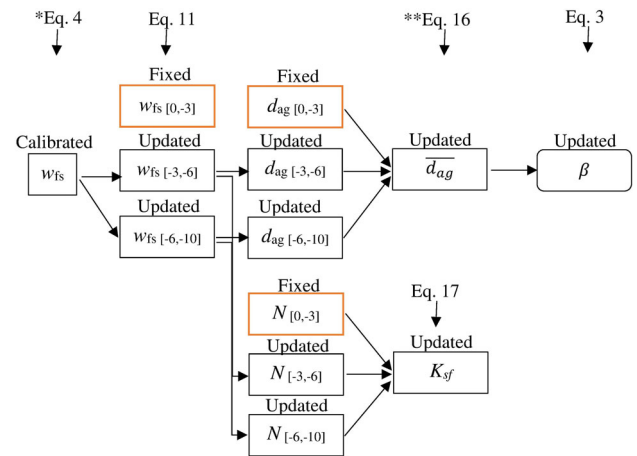
*m and z_{max} were kept fixed to initial measurements

** the flow proportions were kept fixed to initial measurements

FIGURE 3 A tree chart of parameter interaction during calibration of w_{fs}. The parameters with a red box were fixed to initial measurements by disk infiltrometer. The other parameters were updated accordingly after each selection of w_{fs} by the PEST model [Color figure can be viewed at wileyonlinelibrary.com]

TABLE 3 Initial estimation of macropore parameters for HYDRUS 2D/3D at each soil horizon

Depth (cm)	θ_{rf} (−)	θ_{sf} (−)	α_f (cm^{-1})	n_f (−)	K_{sf} (cm min^{-1})	l_f (−)	w_f (−)	β (−)	γ (−)	d_{ag} (cm)	K_a (cm min^{-1})
0–15	0.00	0.80	0.15	2.68	387.08	0.50	7.421E-04	0.63	0.40	2.00	2.66E-02
15–30	0.00	0.80	0.15	2.68	387.08	0.50	7.421E-04	0.60	0.40	2.36	4.92E-03
30–50	0.00	0.80	0.15	2.68	387.08	0.50	7.421E-04	0.55	0.40	3.08	8.63E-03

3 | RESULTS

The relative macroporosity at the soil surface, w_{fs} (Equation (4)), was the only parameter changed in calibration, increasing ~3.5 times relative to its initial measurement. This increase in w_{fs} means that the saturated hydraulic conductivity of the macropores, K_{sf}, and the effective aggregate width, d_{ag}, decreased relative to their initial measurements (Figure 3 and Table 4). The decrease in K_{sf} is explained because we only allow changing $w_{fs[-3,-6]}$ and $w_{fs[-6,-10]}$ during calibration; therefore, the number of smaller diameter macropores increases (see Equation (17)). The physical meaning of d_{ag} is an average distance between the macropore wall and the matrix centre. An increase in w_{fs} after calibration means a higher number of macropores that reduce this distance or d_{ag}. The uncertainty bounds were narrow, indicating a good estimation by PEST (Table 4). The other parameters listed in Table 4 were pegged to w_{fs} during calibration. Consequently, those parameters do not have uncertainty bounds (Table 4).

The cumulative infiltration simulated by HYDRUS 2D/3D from the initial measurements (Table 3) was lower than that measured under field conditions (Figure 4). The Nash Sutcliffe coefficient for that simulation was −0.09. The Nash Sutcliffe coefficient for cumulative infiltration simulated by HYDRUS 2D/3D after the calibration of w_{fs} was 0.88.

The increase of w_{fs} after calibration produces an adjustment in the position of the w_f average (located at depth, g_{zx}; see Equations (12) to (15)) (Figure 5). The subjectively chosen values of the depths $g_{z1} = -15$ cm and $g_{z2} = -50$ cm change after calibration to $g_{z1} = -56$ and $g_{z2} = -74$ cm. Therefore, calibration of w_{fs} updates the arbitrarily chosen depths g_{zx}. Recall that the average relative macroporosity at each depth, g_{z1} and g_{z2}, is computed from the w_f curve generated by the meta-model with Equation (4).

4 | DISCUSSION

4.1 | Initial measurements of meta-model and macropore parameters

Meta-model and macropore parameters (w_{fs}, m, K_{sf}, w_f, d_{ag} and β) were directly obtained over the relevant soil depth from disk infiltrometer measurements, whereas other meta-model and macropore parameters (g_{z1}, g_{z2}, z_{max}, θ_{rf}, θ_{sf}, α_f, n_f, γ, l_f and K_a) were initially guesses that were later updated by calibration (g_{z1}, g_{z2}) or based on previous research. Köhne, Mohanty, and Šimůnek (2006) used similar values for θ_{rf} and θ_{sf} to those used in this research. Gardenas,
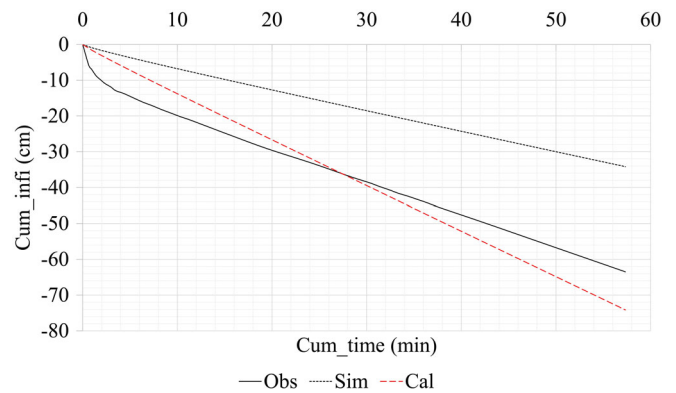

FIGURE 4 Cumulative infiltration measured under field conditions (Obs), simulated with HYDRUS 2D/3D with the initially estimated parameters (Sim), and simulated with HYDRUS 2D/3D after calibration (Cal) [Color figure can be viewed at wileyonlinelibrary.com]

TABLE 4 Initial measurement and calibrated macropore parameters

	Initial	Calibrated	95% lower	95% upper	Units
w_{fs}	0.0013	0.0046	0.0040	0.0052	cm³ cm⁻³
w_f	0.0007	0.0027	*	*	cm³ cm⁻³
K_{sf}	387.08	247.25	*	*	cm min⁻¹
$\beta 1$	0.6261	0.6511	*	*	(−)
$\beta 2$	0.5966	0.6196	*	*	(−)
$\beta 3$	0.5531	0.5733	*	*	(−)
$d_{ag}1$	2.0034	1.8949	*	*	cm
$d_{ag}2$	2.3634	2.2347	*	*	cm
$d_{ag}3$	3.0827	2.9129	*	*	cm

Note: The symbol * indicates a pegged parameter during calibration. Therefore, these do not have 95% uncertainty bounds. w_f corresponds to the average value between 0 and 50 cm. The soil horizons are indicated in the symbols of some parameters by 1 (top), 2 and 3 (bottom).
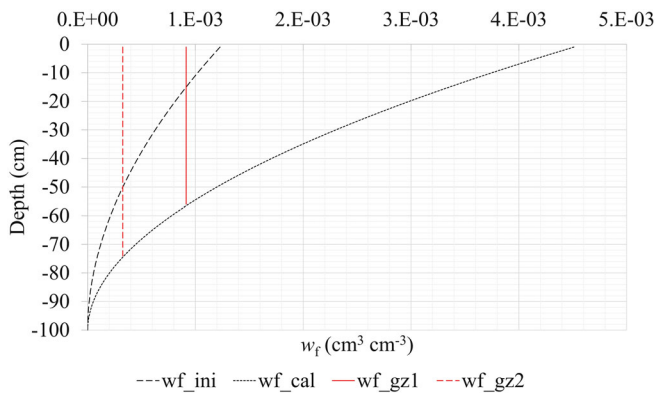
FIGURE 5 Relative macroporosity over depth computed by the meta-model from initial measurements (wf_ini) and after calibration of w_{fs} (wf_cal). w_{f_gz1} and w_{f_gz2} are the average relative macroporosity computed at depths $z_1 = 0$ and $z_2 = 30$ cm, respectively, by disk infiltrometer. The subjectively chosen values $g_{z1} = -15$ cm and $g_{z2} = -50$ cm change after calibration to $g_{z1} = -56$ and $g_{z2} = -74$ cm [Color figure can be viewed at wileyonlinelibrary.com]

Simunek, Jarvis, and van Genuchten (2006) used similar assumptions for the setting of α_f, n_f, γ and l_f with HYDRUS 2D/3D under field conditions. Köhne and Mohanty (2005) and Gerke and van Genuchten (1993) considered the initial setup of K_a equal to the matrix K_s as performed in this research. Therefore, the initial parametrization performed for HYDRUS 2D/3D for the above parameters is concordant with previous research.

We report that HYDRUS 2D/3D simulations were stable. Therefore, the initial macropore parameters previously obtained by the meta-model and previous research (Table 3) are sound for the dual-permeability concept of HYDRUS 2D/3D. This finding is relevant because researchers can apply similar assumptions for setting parameters in HYDRUS 2D/3D.

The average effective macropore width, $\bar{d}_{ag}$, and K_{sf} were weighted proportionally by water flow or number proportion in Equations (16) and (17). We do not know if that is the best way to weight $\bar{d}_{ag}$ and K_{sf} to obtain an accurate initial measurement. Therefore, this is an open topic for future research.

In this research, we only measured the soil hydraulic parameters of the matrix for the top 50 cm of soil. That information was set for the HYDRUS 2D/3D model with a square domain of 50×50 cm and free drainage bottom boundary condition. This implies that the model cannot account for a drastic reduction in infiltration rate when the macropore domain is filled with water.

4.2 | Calibration

The Nash Sutcliffe coefficient obtained from the initial measurements of the meta-model and macropore

parameters by disk infiltrometer data was −0.09. Therefore, calibration was necessary and improved the Nash Sutcliffe coefficient substantially to 0.88. A visual inspection of Figure 4 indicates a mediocre agreement between the calibrated and observed cumulative infiltration curve at the beginning, where a strong capillarity effect is seen. The effect of capillarity forces could have been produced because the sand material utilized was perhaps not fully saturated or simply because of unsaturated matrix flow at the beginning of infiltration. HYDRUS 2D/3D could not reproduce that initial non-linear curve in Figure 4 because we only calibrate one meta-model parameter (w_{fs}) related to macropore flow, with a negligible effect on matrix flow. Additionally, the matrix parameters directly estimated under laboratory conditions by the evaporation method are not error free. Matrix parameters can be calibrated under field conditions using cumulative infiltration from disk infiltrometer data at negative suctions (Kodesova et al., 2010).

The calibration of w_{fs} was tied to other macropore model parameters. Our prior information indicated that water flow is overestimated by the physical assumptions, thereby underestimating w_{fs} and overestimating K_{sf}. The increase of w_{fs} ~3.5 times after automated calibration of the initial value confirms our prior information. Alberti and Cey (2011) utilized the Hagen-Poiseuille equation for the initial measurement of K_{sf}. They also concluded that the initial value is overestimated and should be decreased by manual calibration. The overestimation of macropore flow by the Hagen-Poiseuille equation was previously discussed in Dunn and Phillips (1991) and Watson and Luxmoore (1986).

The final relative macroporosity at the soil surface (w_{fs}) obtained by calibration might still be underestimated. The value of K_{sf} is still high compared to other studies (Arora et al., 2011 or Urbina et al., 2019). However, it is comparable to the one obtained in Alberti and Cey (2011). We think that the high initial value of K_{sf} obtained by Equation (17) influences the calibration of w_{fs}. In other words, starting the inverse estimation with a lower value of K_{sf} would increase the final w_{fs} value obtained by calibration more than ~3.5 times. We performed a calibration of K_{sf}, keeping constant w_{fs} to its initial value (0.0013 cm^3 cm^{-3}; Table 4). The final calibrated value of K_{sf} was 699.2 cm min^{-1} with 95% uncertainty bounds (622.8–784.9) and Nash Sutcliffe coefficient of 0.88. Therefore, a good match between observation and simulations of the cumulative infiltration curve at zero pressure head can be obtained by either increasing w_{fs} or K_{sf}. This indicates that an accurate initial estimation of K_{sf} is necessary to estimate w_{fs} by calibration. In future research, Equation (17) can be modified to include film-flow (Nimmo, 2010) or rivulet flow (Germann et al.,

2007) for macropore diameters higher than 3 mm (Germann, 1987). The previous adjustments would reduce the water flux density and thus reduce the value of K_{sf} compared with the one obtained by Equation (17).

Future field applications should also consider the storage change to improve the calibration with disk infiltrometer data (Šimůnek et al., 1999). The storage change is measured by subtracting the final soil water content after disk infiltrometer infiltration from the initial soil water content. Including the storage change over depth and the measurement of cumulative infiltration at 0 cm pressure head at the soil surface introduce additional information for the calibration of w_{fs} and perhaps would allow calibration of an additional parameter.

Previous studies with HYDRUS advised lumping the parameters related to lateral flow, such as the effective hydraulic conductivity of the fracture-matrix interface (K_a), the scaling factor (γ), the macropore shape (β) and the effective aggregate width (d_{ag}), into one single parameter during calibration (Haws, Rao, Simunek, & Poyer, 2005). Although that solution is practical, it is not easy to provide an initial estimation for the lumped parameter. Additionally, that parameter remains constant over depth; therefore, it cannot represent w_f and d_{ag} variation in heterogeneous macropore geometries. Instead, the meta-model presented here allows finding initial measurements of meta-model parameters by disk infiltrometer data. Moreover, during calibration, the parameters can be tied to other macropore parameters because they are mathematically related.

In this research, we observed only cylindrical macropores for field conditions. The methodology developed in Urbina et al. (2020) details the measurement of w_f for different macropore-matrix geometries such as rings, hexagons, bricks and rectangular slabs using disk infiltrometer data. Therefore, the initial estimation of meta-model parameters can be used for different macropore-matrix geometries, increasing the accuracy of the initial estimation of w_f and d_{ag}.

The feasibility of this research should be analysed in terms of the meta-model and the initial estimation of meta-model parameters by disk infiltrometers. The meta-model included in Equations (4) and (5) and Figure 1 can be used in any inverse estimation for laboratory or field conditions when the number of macropores variates over depth. The initial estimation of meta-model parameters by the disk infiltrometer (Urbina et al., 2020) and its posterior update by inverse estimation (this research) should be used as an initial guess of meta-model parameters for detailed plot studies or risk assessment studies where data for calibration are scarce.

5 | CONCLUSIONS

A meta-model was developed for HYDRUS 2D/3D in the R programming language. The meta-model reduces the number of macropore dual-permeability model parameters needed to simulate field conditions with a vertical variation of the macropore number. The meta-model computes the variation of the relative macroporosity, w_f, and the effective aggregate width, d_{ag}, over depth using only four parameters. The new parameters are the relative macroporosity at the soil surface (w_{fs}), the effective macropore radius (r_m), the maximum depth of macropores (z_{max}) and a shape parameter for the w_f curve (m). All the meta-model parameters have either physical or geometrical meaning; therefore, they can be independently estimated for field conditions. Independent estimation of meta-model parameters is theorized using disk infiltrometer data. The methodology requires data from disk infiltrometer measurements, at least within two depths with different pressure heads, including the 0 cm pressure head.

The previous methodology was applied for field conditions using a disk infiltrometer at two depths for different pressure heads. The initial parameter values of HYDRUS 2D/3D were improved by calibration with the cumulative infiltration data obtained from the disk infiltrometer at the soil surface for a 0 cm pressure head. Only w_{fs} was calibrated because the physical assumptions of the methodology underestimate this parameter and overestimate K_{sf}. The calibration was performed with PEST and was stable. The calibrated value of w_{fs} was ~3.5 times higher than the initial measurement, which is in line with our prior information. We show how the calibration of w_{fs} influenced the values of other macropore parameters, as they are mathematically related. We consider these contributions useful for the initial setup of dual-permeability models to simulate water flow and contaminant leaching in regional risk assessments and detailed plot studies.

AUTHOR CONTRIBUTIONS

Carlos Faúndez Urbina: Conceptualization; formal analysis; methodology; software; visualization; writing-original draft; writing-review & editing. **Jos van Dam:**

Conceptualization; software; supervision; visualization; writing-original draft; writing-review & editing. **Darrel Tang:** Visualization; writing-review & editing. **Harm Gooren:** Data curation. **Coen Ritsema:** Project administration; supervision; visualization; writing-review & editing.

CONFLICT OF INTEREST
The authors have no conflicts of interest to declare.

DATA SHARING AND DATA ACCESSIBILITY STATEMENT
The data are not available for sharing.

SUPPLEMENTARY MATERIAL
In the supplementary material, the computation of initial macropore parameters (Table 3) for HYDRUS 2D/3D is illustrated. Additionally, the initial water content values in the field site are depicted in Figure S2.

DATA AVAILABILITY STATEMENT
The data that support the findings of this study are available from the corresponding author upon reasonable request.

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of this article.