Computers and Geosciences 113 (2018) 33–42

Contents lists available at ScienceDirect

Computers and Geosciences

journal homepage: www.elsevier.com/locate/cageo

Research paper

Modelling soil-water dynamics in the rootzone of structured and water-repellent soils

Hamish Brown [a], Sam Carrick [b], Karin Müller [c], Steve Thomas [a], Joanna Sharp [a], Rogerio Cichota [a], Dean Holzworth [d], Brent Clothier [e,*]

[a] The New Zealand Institute for Plant & Food Research Limited, Lincoln, New Zealand
[b] Landcare Research, Lincoln, New Zealand
[c] The New Zealand Institute for Plant & Food Research Limited, Ruakura, New Zealand
[d] CSIRO, Toowoomba, Australia
[e] The New Zealand Institute for Plant & Food Research Limited, Palmerston North, New Zealand

ARTICLE INFO

Keywords:
Critical zone
Soil-water dynamics
APSIM modelling
Preferential flow
Soil-water repellency
Evapotranspiration

ABSTRACT

In modelling the hydrology of Earth's critical zone, there are two major challenges. The first is to understand and model the processes of infiltration, runoff, redistribution and root-water uptake in structured soils that exhibit preferential flows through macropore networks. The other challenge is to parametrise and model the impact of ephemeral hydrophobicity of water-repellent soils. Here we have developed a soil-water model, which is based on physical principles, yet possesses simple functionality to enable easier parameterisation, so as to predict soil-water dynamics in structured soils displaying time-varying degrees of hydrophobicity. Our model, WEIRDO (**W**ater **E**vapotranspiration **I**nfiltration **R**edistribution **D**rainage run**O**ff), has been developed in the APSIM Next Generation platform (Agricultural Production Systems sIMulation). The model operates on an hourly time-step. The repository for this open-source code is https://github.com/APSIMInitiative/ApsimX. We have carried out sensitivity tests to show how WEIRDO predicts infiltration, drainage, redistribution, transpiration and soil-water evaporation for three distinctly different soil textures displaying differing hydraulic properties. These three soils were drawn from the UNSODA (Unsaturated SOil hydraulic Database) soils database of the United States Department of Agriculture (USDA). We show how preferential flow process and hydrophobicity determine the spatio-temporal pattern of soil-water dynamics. Finally, we have validated WEIRDO by comparing its predictions against three years of soil-water content measurements made under an irrigated alfalfa (*Medicago sativa* L.) trial. The results provide validation of the model's ability to simulate soil-water dynamics in structured soils.

1. Introduction

Earth's critical zone is the “heterogeneous, near surface environment in which complex interactions involving rock, soil, water, air, and living organisms regulate the natural habitat and determine the availability of life-sustaining resources” (National Research Council, 2001). This critical zone is a realm of geoscientific interest because the teeming hydrological processes in this near-surface environment control the quantity and quality of our water resources, as well as the productivity of the vegetation systems, both natural and managed, growing on fractured rocks, and in soils. Furthermore, management of agricultural lands often involves the use of irrigation water, and so understanding and predicting soil-water dynamics in the structured soils of the vadose zone is critical for food production, and also for protecting receiving water bodies from nutrient leaching and runoff losses.

There are two challenges in predicting the soil-water dynamics in the rootzone of structured soils: the preferential transport processes through the macropores (Jarvis et al., 2016); and the widespread and complex temporal variation in the occurrence and severity of hydrophobicity, or soil-water repellency (Müller et al., 2014).

Models, of many types, have been developed, over many years, to enable prediction of water and solute movement through structured soils, and also for transport processes in water-repellent soils. However, few models have considered preferential flow processes in water-repellent soils. Here we describe a model that incorporates both processes simultaneously, and which has been coded in the APSIM (Agricultural

* Corresponding author.
E-mail address: brent.clothier@plantandfood.co.nz (B. Clothier).

https://doi.org/10.1016/j.cageo.2018.01.014
Received 28 July 2017; Received in revised form 17 January 2018; Accepted 21 January 2018

Table 1
Schematic representation of the soil-array structure by pore cohort (*c*) and profile layer (*l*).

		Pore cohort (c)									
		c = 0	c = 1	c = 2	c = 3	c = 4	c = 5	c = 6	c = 7	c = 8	c = 9
Profile layer (l)	l = 0	(0,0)	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)	(0,8)	(0,9)
	l = 1	(1,0)	(1,1)	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)	(1,8)	(1,9)
	l = 2	(2,0)	(2,1)	(2,2)	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)	(2,8)	(2,9)
	l = 3	(3,0)	(3,1)	(3,2)	(3,3)	(3,4)	(3,5)	(3,6)	(3,7)	(3,8)	(3,9)

Production Systems sIMulator) Next Generation platform (Holzworth et al., 2015). Our model is termed WEIRDO (Water Evapotranspiration Infiltration Redistribution Drainage runOff). The repository for this open-source code is https://github.com/APSIMInitiative/ApsimX. Holzworth et al. (2015) note that APSIM Next Gen has a quicker 'time to release' for new models, along with better, more up-to-date documentation and better testing. WIERDO is one of these new models.

1.1. Preferential flow

Long-ranging, preferential flows through the macropores of structured soils have generally been described either by using functional, or mechanistic models. Addiscott (1977) developed a functional model by considering the soil as a stack of slabs, each with two domains: a matrix phase and fast-flowing macropore phase. The macropore domain connected the layers, such that water flowed vertically and/or was absorbed 'sideways' into the matrix. Mechanistic schema have used analytical descriptions to describe the physics of the Richards' flows in dual-domain, and multi-domain models of transport and exchange processes (van Genuchten and Wierenga, 1976; Gerke and Van Genuchten, 1993; Jarvis et al., 2016).

To balance between the restrictive simplicity of functional models and the onerous parametrisation requirements of mechanistic models, we have developed WEIRDO. It is a functional model which enables easier implementation and parameterisation. But it has detailed representation of the soil's porosity and draws its parameters from the soil-water characteristic and hydraulic conductivity function, thereby ensuring a rational physical basis.

1.2. Hydrophobicity

Mechanistic models of the impact of soil-water repellency on soil-water processes have been developed using detailed understanding of the macroscopic dynamics of wetting and drying, and the time-dependency of the contact-angle of wetting in hydrophobic soils (Deurer and Bachmann, 2007). Here in our model for hydrophobicity, we take all of these physical characteristics and we express them in a functional model which enables easy characterisation from the measurements that are normally made to assess water repellency (Wijewardana et al., 2015). Water-repellency was found to widespread across the pastoral soils of New Zealand (Deurer et al., 2011). Our WEIRDO model computes any runoff at the surface by creating a 'surface-pond' of water. This depth of water is then excluded from further infiltration calculations. We have not presented here any simulations dealing with such runoff, which occurs when the applied flux of rain, or irrigation, exceeds the ability of the surface soil's porous system to accept the incident rate. In future, we will connect WEIRDO with a spatially-explicit version of APSIM where will route runoff across the surface according to the depth of the surface pond, the local slope, the surface detention-capacity, and flow resistance.

2. Model structure

Our model, WEIRDO has been developed in the APSIM Next Generation platform to enable easy integration with crop, management and climate modules, and to provide an interface for the easy set-up, execution and visualisation of simulations. It is a layered soil-water balance model designed to capture bypass flow phenomena and the impacts of hydrophobicity, which are often observed but not captured by many soil-water models. Details of the parameters and their calculation, are given in Tables 1 and 2.

2.1. Pore characteristics

The total porosity of each layer is partitioned into cohorts of similar sized pores more cohorts in the near-saturated region (Fig. 1). The movement of water through each cohort of pores is modelled separately. It operates at an hourly time step in most cases but reduces to a 6-min time step when high rates of irrigation or rainfall occur.

2.2. Software structure

The central notion of WEIRDO is that a soil layer's porosity can be grouped into a series of cohorts of similar-sized pores and that the overall behaviour is the result of water movement through each of these pore cohorts. At the top-level, the soil is modelled by WEIRDO.cs which links all processes and collates the pore data-structures. The soil is represented by a two-dimensional array where the first dimension is layers (*l*) in the soil and the second dimension is the pore cohorts (*c*) within the layer (Table 1). Each array member (*l*,*c*) is represented by a generic pore class (Pore.cs) which contains a set of properties defining the parameters of the pore cohort and keeps track of its state.

Each of these properties and their methods of calculation are detailed in Table 2. The only property that is set is the equivalent depth of the water volume stored in each pore cohort (D_W). All other properties are either parameters, set when the model is initialised, or are a function of D_W and/or other parameters. Whenever a process is calculated, WEIRDO.cs will step through each pore class in each layer to determine the changes in the water-in and water-out. The number of pore compartments is fixed in the code at 10 per layer. The soil is sliced into 50 mm layers, and the number of layers (*Nl*) and subsequent profile depth is arbitrary.

2.3. Pore set-up

The model requires the water contents at saturation (θ_S, 0 mm pressure head, ψ), drained upper limit (θ_D, $-1.0e^3$ mm pressure head, ψ), lower limit (θ_L, $-1.5e^5$ mm pressure head, ψ) and air dry (θ_A, $-6.0e^7$ mm pressure head, ψ). A bubbling, or air-entry water potential head, (h_{bub}), is also required, and θ_S is assumed at this potential to give a 5th point to fit (Fig. 1). The scheme assumes boundaries between pore cohorts at pore diameters (d) of 3000, 1194, 475, 189, 75, 30, 8.6, 2.47, 0.707, 0.202 and 0.0005 μm (Fig. 1). So the corresponding water potentials, when all of the pores below these boundaries are water filled (h in mmH_2O), are given by −30000/d (Loll and Moldrup, 2000).

2.4. The hydraulic-flow model

The hydraulic flows in WEIRDO take into account: the vertical gravitational Poiseuille flow governed by the pore's radius which determines its hydraulic conductivity, *k*; the capillary attraction of water due to the pore's sorptivity, *S*; and the impact of hydrophobicity, which is applied only through a reduction factor on the pore's hydrophilic