Mathematical modelling of water and solute movement in ridge plant systems with dynamic ponding

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*Running Title: Solute movement driven by ponding in ridge systems*

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**Highlights**

* Effect of furrow ponding and plant water uptake on solute movement in ridged fields.
* We developed a mathematical model that describes ponding in furrows from rainfall events.
* Solute ‘hot spots’ formed in soil from surface ponding and root water uptake.
* We estimate reduced risk to solute leaching under the effects of ponding when roots are present in soil.

Summary

We present a mathematical model that describes the movement of water and solutes in a ridge and furrow geometry. We focus on the effects of two physical processes: root water uptake and pond formation in the furrows. Special attention is paid to the physical description of ponding as an effect of transient rain events. We focus on phenomena taking place in the furrow cross section, not on the drainage along the furrow. The resulting model comprises of a coupled system of partial and ordinary differential equations that describe the mathematical interplay between solute transport, water movement and furrow pond depth. The system of equations is solved numerically using finite element techniques. We conducted numerical simulations to determine how mobile solutes with low buffer powers penetrate into the soil. We considered two cases; low rainfall, in which pond formation does not occur, and high rainfall, in which significant ponding is observed in the furrows. We found, in the presence of roots, that mobile solutes collected into a concentrated spot adjacent to the root system independent of rainfall intensity. In the absence of roots, however, we observed that water infiltration from ponding acted as the dominant transport mechanism for mobile solutes. This resulted in deep solute penetration into the soil when compared to non-ponded furrows.

Introduction

In arable farming, a specific form of row production known as a ridge and furrow geometry is frequently used to cultivate crops such as potatoes ([Steele *et al.*, 2006](#_ENREF_30)). This geometry is formed when the soil surface is adapted to form a periodic series of peaks and troughs. This allows water to flow across the field providing water to the plants whilst preventing waterlogging of the roots ([Tisdall & Hodgson, 1990](#_ENREF_33)). However, under certain rainfall conditions, this can lead to pond formation in the furrows that can result in decreased yields for crops such as potatoes ([van Loon, 1981](#_ENREF_35)). An understanding of water movement and ponding in ridge and furrow geometries will help in developing strategies for crop and soil management.

There is growing uncertainty about whether ridge and furrow geometries present greater potential for the movement of mobile plant protection products to groundwater than flat fields, because none of the models currently used for regulatory purposes to estimate solute movement to groundwater after application can model this system explicitly ([EFSA, 2013](#_ENREF_11)).  Consequently, a universal multiplier has been proposed to extrapolate between estimates of residues calculated for flat fields and those in ridge and furrow geometries ([EFSA, 2013](#_ENREF_11)).  In the absence of extensive and expensive field data, mathematical models designed to model solute movement explicitly in ridges and furrow geometries can provide insight into understanding the effects of ponding in these systems.

Mathematical modelling of water movement in ridge and furrow systems has been studied increasingly in recent years ([Ebrahimian *et al.*, 2013](#_ENREF_10); [Bautista *et al.*, 2014](#_ENREF_6); [Sanchez *et al.*, 2014](#_ENREF_27)), often for semiarid soil where the ridge and furrow geometry is used to facilitate irrigation. Because of the lack of rain in these environments, precipitation and surface runoff are often disregarded because furrow irrigation management is the main priority.

In this paper, we develop a general mathematical model for solute movement in ridge and furrow soil, taking account of surface ponding and water movement from transient rainfall events to understand how solutes move in United Kingdom environments. We consider the movement of water and solutes in temperate soils with no formal irrigation, but subjected to substantial rain that results in ponding on the soil surface. The model presented can then be customized for specific fertilizers or pesticide-like solutes by including other soil processes such as biodegradation, microbial mineralization and air volatilization to determine how a particular solute will behave under a specific rainfall regime.

Several models for pond infiltration have been presented in the literature ([Ebrahimian *et al.*, 2013](#_ENREF_10); [Bautista *et al.*, 2016](#_ENREF_5)). However, these models describe irrigation and drainage longitudinally along a furrow (often using the zero-inertia model for a moving body of water). To describe dynamic ponding from transient rainfall events, we developed a model that captures the filling and draining of a pond on the soil surface. In addition, we consider root water uptake in the ridges of the geometry. We assess soil ponding from a mechanical perspective and incorporate Dirichlet and flux boundary conditions to represent areas of ponding and water free surfaces, respectively ([Camporese *et al.*, 2010](#_ENREF_9)). We shall disregard fluid drainage along the length of the furrow because our main concern is ponding from rainfall, rather than irrigation that transports water down the furrow.

To study the effects of solute movement under the influence of surface ponding, we coupled water movement with solute transport in soil. We incorporated the movement of solutes into the model to understand better how nutrients, fertilizers and pesticides move under the effect of surface ponding in the presence and absence of roots. The physical characteristics of solutes can lead to adverse effects on the local environment, however, mathematical modelling enables us to develop strategies to reduce these negative effects by either aiding or impeding solute penetration into the soil, i.e. to promote the movement of low mobility fertilizers or to reduce the leaching of high mobility solutes.

Previous modelling of ridge and furrow system behaviour typically used software packages such as HYDRUS-2D, WinSRFR and so on ([Ebrahimian *et al.*, 2013](#_ENREF_10); [Sanchez *et al.*, 2014](#_ENREF_27); [Bautista *et al.*, 2016](#_ENREF_5)). Although they enable easy implementation of fluid flow models, we chose to use general finite element software (COMSOL Multiphysics®, Stockholm, Sweden, [www.comsol.com](http://www.comsol.com)) because it allows us to generalize fluid flow and surface ponding. It provides greater flexibility and easier implementation of new physics without relying on the functionality of software.

Our model presented in this paper consists of a coupled system of two partial differential equations (PDEs): one for the movement of water in soil and one for the transport of solutes. We also introduce an additional ordinary differential equation (ODE) that is coupled to the system of PDEs to describe dynamic ponding. It should be noted that we disregard any effects of soil moisture from heat transfer in soil because our focus is surface ponding and soil waterlogging in a temperate UK environment.

Mathematical model

In this section, we derive a model for simultaneous water and solute movement in variably saturated soil that accounts for the ridge and furrow geometry and the effects of dynamic surface ponding. The movement of solutes in soil is known to depend considerably on the degree of water saturation ([Nye & Tinker, 1977](#_ENREF_21)). Therefore, we constructed a coupled water and solute movement model to connect soil water pore pressure with solute concentration. We assume that solutes do not create osmotic pressure gradients that influence fluid flow, i.e. fluid flow influences solute movement, but not *vice versa*.

The symmetry and periodicity of the ridge and furrow structure enables us to describe the complete system with a single half-period of the ridge and furrow geometry. The geometry used in this study is shown in Figure 1 by the domain, which was chosen to be consistent with the dimensions for typical ridge and furrow geometries ([Steele *et al.*, 2006](#_ENREF_30); [Li *et al.*, 2007](#_ENREF_16)). We approximate the soil surface (see Figure 1) by the periodic function,

|  |  |  |
| --- | --- | --- |
|  |  | (1) |

where is the variation in soil depth, is the ridge wave number and is the average soil depth.

*Water movement in variably saturated soil*

To describe water movement in ridged soil systems, we assume there may be regions of soil that are fully saturated (i.e. directly under the pond) and regions that are partially saturated. To account for this, we constructed a model that can switch between a partially and a fully saturated soil environment with a moving interface between the two regions.

For water movement in variably saturated soil, Richards’ equation is used ([Kollet & Maxwell, 2006](#_ENREF_14); [Weill *et al.*, 2009](#_ENREF_38)). This equation is derived by combining the equation for mass balance of soil water flow ([Richards, 1931](#_ENREF_23)),

|  |  |  |
| --- | --- | --- |
|  | ,, | (2) |

with Darcy’s law,

|  |  |  |
| --- | --- | --- |
|  | . | (3) |

The result is Richards’ equation in mixed form,

|  |  |  |
| --- | --- | --- |
|  | , | (4) |

where is the soil porosity, is the relative saturation (i.e.,where is the volumetric water content), is the volume flux of water, is the relative hydraulic permeability, is the viscosity of water, is the soil water pore pressure, is the density of water, is the acceleration due to gravity, is a unit vector in the upwards direction and is a sink term which describes water uptake via plant roots.

The root water uptake function, , is given by the difference in soil water pore pressure and the pressure in plant roots ([Roose & Fowler, 2004a](#_ENREF_24)) and is assumed to be active only where roots are present. We split into two regions, is the zone in which roots take up water and is the region in which there are no roots. Hence, we write,

|  |  |  |
| --- | --- | --- |
|  | , | (5) |

where is the product of the root surface area density and water conductivity of the plant root cortex and is the pressure in the root xylem.

We express as a function of using the van Genuchten pressure-saturation relation ([van Genuchten, 1980](#_ENREF_34)) (also called the suction characteristic),

|  |  |  |
| --- | --- | --- |
|  | ,  | (6) |

where is the atmospheric pressure, is the characteristic suction pressure and is a van Genuchten parameter. The parameters and are determined experimentally for each soil ([van Genuchten, 1980](#_ENREF_34)). Note that we choose to set, such that is defined as the gauge pressure relative to the atmospheric pressure ([Roose & Fowler, 2004a](#_ENREF_24)).

To describe the relative permeability , we used a second van Genuchten formula ([van Genuchten, 1980](#_ENREF_34)),

|  |  |  |
| --- | --- | --- |
|  | , | (7) |

where is the saturated hydraulic permeability.

Combining Richards’ Equation (4) with the van Genuchten Equations (6)–(7) ([van Genuchten, 1980](#_ENREF_34)), we can write the water movement model in terms of only:

|  |  |  |
| --- | --- | --- |
|  | , | (8) |

where,

|  |  |  |
| --- | --- | --- |
|  |  | (9) |

and

|  |  |  |
| --- | --- | --- |
|  | . | (10) |

Richards’ equation is frequently used to describe water movement in partially saturated soil. However, we can adapt Equations (8)–(10) such that it can represent both a saturated and partially saturated soil. To adapt Richards’ equation for variably saturated soil, we use similar methods to those used previously by others ([Kollet & Maxwell, 2006](#_ENREF_14); [Weill *et al.*, 2009](#_ENREF_38); [Bautista *et al.*, 2014](#_ENREF_6)) that reduce Richards’ equation to saturated Darcy flow in the event of full saturation (for ). We do this by modifying Equations (8)–(10) in two ways. First, for we eliminate the term from Equation (8) by setting, which in turn reduces Richards’ equation to Darcy flow. Thus, to describe the movement of water in variably saturated soil, we impose the condition:

|  |  |  |
| --- | --- | --- |
|  | . | (11) |

To implement Equation (11) as a closed-form expression, we use a smoothing approximation to the Heaviside function to set as. This imitates the piecewise Equation (11) while retaining a level of smoothness over a narrow transition region about to aid in numerical simulation. We add the smoothed Heaviside function, such that

|  |  |  |
| --- | --- | --- |
|  | , | (12) |

where

|  |  |  |
| --- | --- | --- |
|  | , | (13) |

and defines the width of transition between and around.

Second, when Richards’ equation is reduced to Darcy flow, the function is required to be constant in the fully saturated soil regime. Thus, we introduce a second condition,

|  |  |  |
| --- | --- | --- |
|  | , | (14) |

where is a small transition pressure that acts as the interface between the saturated and partially saturated soil regions. We introduced to avoid discontinuities in the numerical solution to Equation (12). These discontinuities come from the second term in Equation (12) because we need evaluate. However, is singular at the transition between fully and partially saturated soil, such that. Hence, we introduce such that is never evaluated. If we did not do this, the numerical procedure would fail to converge. The parameter differs from because is applied strictly to the negative side of, whereas smooths either side of the pressure.

*Soil surface boundary condition*

To form a complete description of the ridge and furrow system, we derive boundary conditions that are imposed on the edges of, and a novel and original ODE for a moving surface point interface for dynamic water ponding on the soil surface that is coupled to Richards’ equation for water infiltration into soil.

To represent ponding, which is often present in ridge and furrow systems ([Tabuada *et al.*, 1995](#_ENREF_32); [Vogel *et al.*, 2000](#_ENREF_36)), we split the boundary (see Figure 1) into two distinct regions. This is shown in Figure 2, where is the surface of soil that is not ponded, i.e. where rain penetrates the soil directly, and is the region on which ponding occurs. Note that we allow the point connecting and to move in time, i.e. , such that the pond height can change transiently.

We assume the pond boundary condition on can be represented by a hydrostatic boundary condition ([Tabuada *et al.*, 1995](#_ENREF_32); [Vogel *et al.*, 2000](#_ENREF_36); [Kollet & Maxwell, 2006](#_ENREF_14)). On the soil surface directly under the pond, we apply the pressure that results from the height of the water column in the pond above it, i.e.

|  |  |  |
| --- | --- | --- |
|  |  | (15) |

where is the depth of the pond.

Precipitation landing on the bare soil enters the soil domain by a combination of capillary forces and gravitational effects. Therefore, we implement a normal fluid flux condition on ([Yang *et al.*, 1996](#_ENREF_40)), such that

|  |  |  |
| --- | --- | --- |
|  | , | (16) |

where, is the unit normal vector pointing outwards from , is the volume flux of water per unit area of soil surface ,i.e. rain, is the infiltration capacity of the soil, and is the volume flux of water entering the soil per unit surface area. In the event of sufficiently heavy rain, the quantity of water that can enter the soil system is limited by the infiltration capacity of the soil. Any excess rain that exceeds, i.e. is defined as the surface runoff , and is quantified by:

|  |  |  |
| --- | --- | --- |
|  | , | (17) |

where is the generalized curve of, given by Equation (1).

To determine the change in pond depth for the boundary conditions imposed on and, we implement an additional ODE that is coupled to the governing water movement model, Equations (12)–(14). This connects the volume of water in the pond, the rate of rainfall, the surface runoff and the flux entering the soil domain from the pond, i.e. the quantity of water leaving the pond and infiltrating into the soil.

We define the maximum depth of the pond (see Figure 2) at a given time to be:

|  |  |  |
| --- | --- | --- |
|  | , | (18) |

where is the co-ordinate at which the pond starts, i.e. the partition between and. It should be noted that for to have this definition, the vertical datum is measured from the base of the soil curve (see Figure 2). This allows the hydrostatic boundary condition Equation (15) to be re-written such that

|  |  |  |
| --- | --- | --- |
|  |  | (19) |

where .

In addition, a length is chosen to represent half a ridge and furrow period (see Figure 2). It follows that for a given pond volume, the partition of the pond boundary is calculated by,

|  |  |  |
| --- | --- | --- |
|  | . | (20) |

The change in pond volume is defined to be

|  |  |  |
| --- | --- | --- |
|  | , | (21) |

where is the rainfall entering the pond, is the surface runoff and is the quantity of water leaving the pond and infiltrating into the soil by the boundary condition on Equation (19) ([Wöhling & Schmitz, 2007](#_ENREF_39)). We substitute Equation (20) into Equation (21) such that

|  |  |  |
| --- | --- | --- |
|  | , | (22) |

where is defined by Equation (18). Equation (22) describes the change in the position of the pond boundary, given the rainfall entering the pond, surface runoff and water infiltration from the pond into the surrounding soil. To calculate, Equation (22) is coupled with Richards’ equation by Equations (12)–(14) and the boundary condition Equation (19).

Through successive application of the Leibniz integral rule and the chain rule, for the generic function, Equation (22) can be expressed explicitly as a function of, i.e.

|  |  |
| --- | --- |
|  . | (23) |

Note that for the boundary condition on, Equation (19), to be active, we impose the condition that a minimum pond depth threshold must be reached before water leaves the pond and infiltrates into the soil:

|  |  |
| --- | --- |
| , | (24) |

where is the minimum pond depth. We impose this condition to aid numerical computation because a pond that is much smaller than the mesh size can lead to convergence problems for the numerical solver. However, we chose the threshold to be sufficiently small that it has a negligible effect on the results.

*Lateral boundary conditions*

For the boundaries and, we set a zero flux boundary condition:

|  |  |  |
| --- | --- | --- |
|  | . | (25) |

Therefore, there is no lateral water movement into or out of .

*Boundary condition at the base of the soil*

For the boundary at the base of the domain, we set a Dirichlet boundary condition ([Banti *et al.*, 2011](#_ENREF_3)). This describes a constant saturation level at a constant depth, i.e. below (see Figure 2). Thus, we impose the condition,

|  |  |  |
| --- | --- | --- |
|  |   | (26) |

*Initial conditions*

For the initial pressure condition, we impose the steady state pressure profile that forms when roots are not present:

|  |  |  |
| --- | --- | --- |
|  | . | (27) |

Furthermore, we assume there is no surface ponding present on at,

|  |  |  |
| --- | --- | --- |
|  | , | (28) |

such that the pond depth is.

The system of Equations (12), (14), (16), (19), (23)–(28) completes the description of the coupled water balance in the presence of surface ponding.

*Solute movement in variably saturated soil*

In this section, we introduce a mathematical model for solute movement in soil. We couple it with the water movement model derived above, thereby constructing a model for simultaneous water and solute movement in soil. The model is coupled by a similar approach to that used by Roose & Fowler ([2004b](#_ENREF_25)). It should be noted that we assume that there is no solute uptake by plant roots or degradation of the solute from other soil processes. Here we deal only with the solute transport problem of solutes that are not actively taken up by plant roots, although it is trivial to customize and extend the model to accommodate solute uptake by plant roots or other soil processes. Examples of passive solutes include non-ionic strongly lipophilic substances, which are taken up minimally by barley (*Hordeum vulgare* L.) plants because of their lipophilicity ([Briggs *et al.*, 1982](#_ENREF_7); [Briggs *et al.*, 1983](#_ENREF_8)).

To model the movement of solutes in soil, we use the advection–diffusion equation ([Nye & Tinker, 1977](#_ENREF_21); [Barber, 1995](#_ENREF_4)):

|  |  |  |
| --- | --- | --- |
|  | , | (29) |

where is the solute diffusion coefficient in the soil pore water, is the volumetric water content, is the solute concentration in the pore water,is the volume flux of water and is the buffer power of the solute. We assume to be constant in this model. However, it is trivial to extend to more complex adsorption isotherms, i.e. Langmuir or Freundlich.

The volumetric water content is related to the soil water pore pressure by the suction characteristic. In addition, we state that in Equation (29) is described by Darcy’s law, as in the water movement model, Equation (3). Finally, we assume can be expressed by the power law

|  |  |  |
| --- | --- | --- |
|  | , | (30) |

where is the diffusion coefficient in free liquid and is the impedance factor of the solute that accounts for the tortuosity of the solute moving through the soil pore space ([Nye & Tinker, 1977](#_ENREF_21)).

Combining Equations (29) and (30) with Equations (12)–(14) that govern water movement, the model for solute movement is given by,

|  |  |  |
| --- | --- | --- |
|  |  . | (31) |

Note that for the solute model to be valid for a variably saturated soil domain, a similar condition to Equation (14) has been imposed. This condition sets the ‘time’ coefficient, the diffusion coefficient and the advection coefficient to be constant at full saturation. Thus, these coefficients do not change under different magnitudes of pressure in a fully saturated environment.

The solute model Equation (31) is coupled to the water movement model, Equations (12)–(14) to achieve a system of PDEs that describes simultaneous water and solute movement in soil.

*Soil surface boundary condition*

For the application of solutes to a soil surface, we assume that this would be during dry conditions or when rainfall is sufficiently low that it does not break the minimum pond depth. Therefore, on the boundary we impose a flux condition similar to Equation (16) such that

|  |  |  |
| --- | --- | --- |
|  | , | (32) |

where is the volume flux of solute per unit soil surface area per unit time entering the soil domain.

*Lateral boundary conditions*

For the boundaries and on the lateral sides of the domain (see Figure 1), we set a zero flux boundary condition:

|  |  |  |
| --- | --- | --- |
|  | . | (33) |

Therefore, there is no lateral solute movement into or out of .

*Boundary condition at the base of the soil*

During our numerical simulations, we observed that the domain was sufficiently large to avoid any solute reaching the base. Therefore, we can implement either a zero flux boundary on or a Dirichlet boundary corresponding to the initial condition. The choice is inconsequential given that any solute movement in numerical simulations is contained in the top of the geometry. Therefore, we impose a zero flux condition:

|  |  |  |
| --- | --- | --- |
|  | . | (34) |

To validate the zero flux condition, we checked that there was zero solute concentration on throughout the numerical simulation, i.e. no solute reaches the base of .

*Initial conditions*

We aimed to observe the effect of ponding on solute movement in previously solute free soil. Therefore, we impose a uniform zero initial concentration across with:

|  |  |  |
| --- | --- | --- |
|  | . | (35) |

Parameter values

There are 24 parameters in the model derived in the section above. These parameters are; , , , , , , , , , , , , , , , , , , andfor the coupled model, and the four parameters,, and for the construction of . These parameters are summarized in Tables 1 and 2.

*Geometric, soil, environmental, plant and solute parameter values*

To replicate the dimensions of ridge and furrow geometries, we used the values, and ([Steele *et al.*, 2006](#_ENREF_30); [Li *et al.*, 2007](#_ENREF_16)). Furthermore, potato (*Solanum tuberosum*, L) is shallow rooted with the majority of its roots in the plough layer, i.e. the top of soil ([Lesczynski & Tanner, 1976](#_ENREF_15)). Therefore, we chose the size of the soil root region to be the top of soil extending radially from the top of the ridge (see Figure 1).

Several of the model parameters depend on the soil, for example and ; the values of these for several soil types are listed in Table 1 ([van Genuchten, 1980](#_ENREF_34)). Potatoes are frequently grown in ridge and furrow geometries of silt loam soil ([Ahmadi *et al.*, 2011](#_ENREF_1)). Therefore, we used the parameter values for the ‘Silt Loam G.E.3’ soil from Table 1, i.e., , and ([van Genuchten, 1980](#_ENREF_34)).

We took values from literature for the environmental and fluid parameters. For the viscosity of water we used ([Watson *et al.*, 1980](#_ENREF_37)), for acceleration due to gravity and for the density of water .

The typical range of the impedance coefficient is between 0.5 and 2 ([Nye & Tinker, 1977](#_ENREF_21)); an increase in volumetric moisture content leads to an increase in impedance factor ([Rowell *et al.*, 1967](#_ENREF_26)). Given that we aimed to simulate surface ponding with fully saturated soil near the surface of the geometry, we used .

Values of the diffusion coefficient of a solution in free liquid, for simple electrolytes tend to be within the range of ([Shackelford & Daniel, 1991](#_ENREF_28)); we used a value in the middle of this range, .

For the parameters in the water root uptake term,, and, we selected typical values for potato plants. The parameter is the product of the root surface area density and water conductivity of the root cortex, which can be expressed by:

|  |  |  |
| --- | --- | --- |
|  | , | (36) |

where is the root length density and is the radial conductivity of root cortex per unit root length. For the root length density, we assigned the value ([Kirkham *et al.*, 1974](#_ENREF_13); [Lesczynski & Tanner, 1976](#_ENREF_15)). In maize (*Zea mays* L.) roots, the parameter is given the value ([Roose & Fowler, 2004a](#_ENREF_24)). Maize and potato roots have been found to have similar root radii ([Rawsthorne & Brodie, 1986](#_ENREF_22); [Steudle *et al.*, 1987](#_ENREF_31)), therefore, we assume that this value of is also representative of potato roots in soil. This leads to the parameter value.

 To describe root pressure , there are models for the root pressure distribution within a single root ([Roose & Fowler, 2004a](#_ENREF_24)). To simulate large areas of soil consisting of many roots, therefore, we used an average root pressure to describe the plant root system. The root pressure can vary considerably in potatoes depending on several factors including soil saturation and atmospheric conditions ([Gandar & Tanner, 1976](#_ENREF_12)). Liu *et al.* ([2006](#_ENREF_17)) found that the root water potential changes substantially based on the method of irrigation applied to the crop. A value of was present in the roots for a fully irrigated system and of for areas of soil with partial root drying. Given that we aimed to model frequent heavy rain events that promote considerable ponding, we chose the values and depending on the simulated rainfall regime (see *Rainfall, infiltration capacity and solute application parameters* for the applied rainfall regimes).

For the parameters and, we selected small values that have a negligible effect on the numerical solution; for we chose . Given that pressure in soil is often measured in , we assumed that was sufficiently small to avoid affecting the numerical results. Furthermore, for which determines the minimum pond depth, we chose . Therefore, the hydrostatic boundary condition Equation (19) is activated once the pond depth surpasses.

For the parameter in the smoothed Heaviside function, we assigned ; this limits the width of the transition between partially and fully saturated soil regions such that the transition is completed across. We conducted a series of simulations for decreasing values of to determine when differences between results became negligible. We tested and confirmed that this value had a negligible effect on numerical computation given that soil water pore pressure is typically several orders of magnitude higher than .

We ran several numerical simulations for a mobile solute to determine how ponding and root water uptake affect the transport of mobile solutes in soil. For this we selected a buffer power of . Examples of solutes with a similar buffer power include the nutrient boron ([Barber, 1995](#_ENREF_4)), and the pesticide Dimethylamonium chloride ([Njoroge *et al.*, 2016](#_ENREF_19)).

*Boundary and initial condition parameters values*

We assigned values to the remaining parameters in the boundary and initial conditions to complete the system of equations that makes up the solute ponding model.

For , which describes a constant saturation at the base of the geometry, we assigned a value of This equates to a saturation level of approximately for a silt loam soil, thereby replicating a shallow water table. For the initial condition of soil water pore pressure,, we chose the steady state profile that forms in the absence of plant roots. As a result of capillary forces and gravity, this leads to a constant pressure gradient from the base to the top of the geometry of:

|  |  |  |
| --- | --- | --- |
|  | , | (37) |

where and .

*Rainfall, infiltration capacity and solute application parameter values*

Here we describe the solute application and rainfall regime used in the numerical simulations. There are several case studies that could be examined with varying solute applications, rainfall events, infiltration capacities and so on, therefore, it is not possible to cover an exhaustive series of case studies. We chose a series of scenarios to observe the effects surface ponding and root water uptake from vegetation have on the transport of mobile solutes in soil.

We simulated solute and water movement over a 16-week period because this timeframe is typical of a single season potato crop ([Noda *et al.*, 1997](#_ENREF_20)). To observe the effect of water uptake from plant roots and ponding on the soil surface, we simulated heavy and light rain both with and without roots for a mobile solute; four simulations in total. The rainfall regimes are shown in Figure 3.

In the light rainfall regime (Figure 3), we simulated one rain event every week (midweek) throughout the 16-week period that lasted 4 hours and had an intensity of . This is not sufficient to generate soil surface ponding because all rainfall infiltrates into the soil. In this case we imposed a root pressure of because this quantity of rainfall will result in a drier soil than with the heavy rainfall regime.

For heavy rainfall (Figure 3), we simulated a rain event every week (midweek). In weeks 1, 3 and 4 we simulated a rain event that lasted 4 hours with an intensity of, and in week 2 we simulated an event that lasted 4 hours with an intensity of 12.5 . This heavier rain caused ponding in the furrows of the geometry. This 4-week routine was repeated throughout the simulation. For heavy rain we imposed a root pressure of because ponding saturated the soil.

The infiltration capacity of soil is known to depend on several factors including tillage methods ([Azooz & Arshad, 1996](#_ENREF_2)), volumetric water content, soil type and recent rain events. Therefore, it is difficult to assign a single value to the infiltration capacity of a soil. Morin & Benyamini ([1977](#_ENREF_18)) found that steady state infiltration of bare loam soil was reached after approximately 20 minutes into a rain event. Given that we simulated rain events an order of magnitude longer than this, we assigned a constant value for the infiltration capacity. Morin & Benyamini ([1977](#_ENREF_18)) found the steady state infiltration rate of bare loam soil is between . Given this, we assigned a value of .

At the beginning of the simulation, a solute was applied to the soil surface over a period of 24 hours, with a total application of, an application rate of.

Numerical Solutions

Before we consider the two rainfall scenarios described above we validated the model first with previous data from ponding in ridge and furrow geometries.

*Model validation*

We validated the model with data from the ponding study by Siyal *et al.* ([2012](#_ENREF_29)). They created a trapezoidal ridge and furrow geometry with a loam soil in which a constant flow of water flowed longitudinally down the furrow until a pond height of was reached. Once the desired pond height was reached, the flow of water was stopped and the time required for the pond to infiltrate fully into the soil was measured.

The model derived in this paper uses a sinusoidal curve to model the periodic surface of ridge and furrow structures. It is impossible to resolve a piecewise trapezoidal surface with the sinusoidal surface Equation (1). Nevertheless, we constructed a geometry with Equation (1) that minimizes the differences between the trapezoidal structure in Siyal *et al.* ([2012](#_ENREF_29)). This was achieved with the geometry parameters, and for the soil surface in Equation (1).

In Siyal *et al.* ([2012](#_ENREF_29)), the time taken to generate the 0.1-m deep pond was 5.6 hours, and the time required for the water to infiltrate fully into the soil was hours. To replicate these conditions, we simulated a rain event that lasted 5.6 hours with an intensity of to equate the total pond volume in the simulated sinusoidal geometry with that of ponded water in Siyal *et al.* ([2012](#_ENREF_29)).

We conducted a simulation to measure the time required for the pond to infiltrate the soil fully with the parameters estimated experimentally for the soil used in Siyal *et al.* ([2012](#_ENREF_29)), i.e. *,*  (assuming the fresh water properties , and ), and . We used the COMSOL Multiphysics® finite element package to solve our model (implementation of the model is described in the Appendix).

In the numerical simulation, we found that the pond caused by the 5.6-hour rain event dissipated into the soil fully after approximately hours. This led to a difference of between these results with the model derived in this paper and those of Siyal *et al.* ([2012](#_ENREF_29)).

These results give us confidence that the model derived in this paper can accurately describe time variable ponding for loam soil.

*Saturation results*

Figure 4 shows the effect of ponding on the water profile of the ridged domain by a series of plots within the domain, for the first ponding rain event from the simulation with the heavy rainfall regime and in the absence of plant roots. The times chosen were selected to emphasize the formation, growth and dissipation of a pond in the furrow. Note that each plot in Figure 4 has a different colour scale bar. Because large soil pore water pressure differences form throughout the simulation, the saturation gradients that result from ponding would otherwise be reduced in appearance if the scale considered both low and high saturation when a ponding event was present.

Figure 4 (a–c) shows the water distribution before, during and at the end of the first rain event, respectively. Figure 4 (d–i) shows the water profile within the soil domain after the rain has finished, showing the effect of surface ponding on the water movement in the soil.

At the start of the rain event, (Figure 4a), we observe steady state conditions that are formed from the boundary conditions imposed on the domain. This causes a constant pressure gradient to form throughout the geometry in which the base of the soil is the most saturated. As the rain starts, we can see the effect of the rain in the top of the soil domain. At hours after the rain starts (Figure 4b), a pond has formed in the furrow of the domain. This equates to a pond depth of approximately 4 cm. During the remaining rain the pond steadily increases to a maximum height of approximately 7 cm.

Once the rain has stopped, the effect from surface ponding becomes evident. Figure 4(d) shows that six hours after the rain saturation in the ridge of the geometry has decreased as the non-ponded soil begins to drain. However, the furrow is still fully saturated as the pond on the soil surface gradually infiltrates into the soil. The pond on the surface continues to infiltrate for approximately 24 hours. The ponding effect on the water profile is shown in Figure 4(e,f) for hours after the rain, respectively. These plots show the diminishing size of the pond and movement of water from the top of the geometry to the base. The soil in the ridges of the geometry has dried considerably faster than in the furrows; this is to be expected given the effect of surface ponding.

Thirty-six hours after the rain event (Figure 4g), the pond has fully infiltrated the soil and the water profile is returning to equilibrium. Two weeks after the rain event (Figure 4i), a steady state equilibrium is achieved in the system. This water movement cycle is then repeated for the second, third and fourth ponding rain events for the remaining simulation.

*Solute transport results*

Figure 5 shows the solute concentration profiles within for the mobile solute (with buffer power) at the end of the 16-week simulations for different rainfall regimes and root water uptake. There were four combinations of rainfall intensity (ponded and non-ponded), and root presence in the ridges of the domain. The solute profiles at the end of the 16-week period are markedly different in each of the four cases.

Figure 5(a) shows the combination of ponded rain without root presence. The effect of ponding in the furrow is clear, and the solute adjacent to the furrow has penetrated much deeper into the soil than that in the ridge. The shape of the solute profile in the furrow corresponds to the fully saturated region of soil that was displayed in Figure 4 because infiltration of water from the pond acts as a carrier mechanism for the solute. Because the soil has a given infiltration capacity, the ridge of the domain can absorb a finite amount of water only, excess water enters the pond. This causes the solute near the ridge to move fairly uniformly into the soil.

The results in Figure 5(a) are quite different from those in Figure 5(b) for the non-ponded rain without roots. Because all of the rain infiltrated the soil, the solute penetrates almost uniformly. However, there is a larger concentration of solute in the ridge of the domain. After a rain event, the first region of soil to dry out is the ridge of the geometry (Figure 4). Because solute movement depends on the saturation conditions, this reduction in relative saturation causes a decrease in movement of the solute in the ridge of the geometry. Therefore, any solute contained in the ridge after drying has occurred, remains there until the succeeding rain event.

Figure 5 (c,d) shows the solute profiles for the heavy and light rain events with roots present in the ridge of the geometry. For both regimes, we imposed root pressures of and , respectively, to account for the difference in available water to the plant roots. In both cases, the solute collects into a concentrated spot at the edge of the root domain. This is caused by the difference in soil pore water pressure and the pressure in the root xylem because any water that infiltrates the soil surface is drawn towards the plant roots, which acts as a carrier mechanism for the solute movement. Therefore, solute in the furrow of the domain is transported to the root system resulting in the formation of a concentrated solute spot.

Figure 5(d) shows a more concentrated and condensed spot formation in the light rainfall regime. This is because of the greater pressure difference between the soil pore water pressure and the pressure in the root xylem, and the reduction in available water. This reduces the diffusion of the solute and forms a more concentrated spot. In the heavy rainfall regime a spot with greater saturation has formed. This enables a larger rate of diffusion resulting in increased dispersion of the solute.

Figure 5(c) still shows the effects of ponding on the soil surface. As the quantity of water overcomes the pressure gradient between the soil and plant roots, this causes a fraction of the solute to penetrate deep into the soil. However, the quantity of solute that penetrates deep into the soil is greatly reduced compared to the simulation without plant roots (Figure 5a).

Conclusions

We developed a coupled system of PDEs that describe the movement of water and solutes in soil. Furthermore, we incorporated an ODE to represent dynamic ponding as a function of rainfall, surface runoff and infiltration of water from a pond into the soil. We validated the pond model using data from a ridge and furrow study that measures the infiltration time of a pond into a loam soil, and found a difference only between the results of the study and model simulations.

We found that when roots are absent in ridge and furrow soils, ponding can have a considerable effect on the penetration of solutes that are applied in the furrow of the geometry. This is directly affected by the size of the pond that forms in the furrows, which results from the quantity of rainfall and infiltration capacity of the soil. As the infiltration capacity of the soil decreases, the total volume of water immediately infiltrating the soil decreases and generates a larger pond in the furrow. This leads to a greater quantity of water infiltrating into the furrow, and transporting the solute deep into the soil. This can lead to deep solute penetration, which can cause substantial solute leaching.

The effects of solute penetration can be reduced by the presence of plant roots in the ridges of the domain. With the addition of vegetation to the ridges of the soil, the movement of water was dominated by the pressure gradient between the soil pore pressure and the pressure in the root xylem. Hence, the majority of infiltrated water from rainfall or ponding is moved towards the plant roots in the ridges of the system, which led to solutes collecting adjacent to the root system. This could substantially reduce the quantity of solutes that move deep into the soil with heavy rain and surface ponding. Knowledge of this solute movement mechanism can aid targeted solute application on ridged surfaces to avoid leaching and contamination, as well as promoting crop yields in which solute application can be directed to provide greater efficiency for crops and plants.

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Appendix: Numerical solution of the model with COMSOL Multiphysics

Here we describe how we used COMSOL Multiphysics (Version 5.1) finite element package to solve the model derived in this paper. We implemented the coupled system of PDEs for simultaneous water and solute movement, with the addition of an ODE for dynamic ponding on the soil surface.

*Coupled water and solute model*

We used COMSOL’s inbuilt ‘General Form PDE’ to set up the coupled system of PDEs, Equations (12) and (31). This takes the form:

|  |  |  |
| --- | --- | --- |
|  |  | (38) |

where and , , and are parameters to be defined by the user. To write the model in this form, the parameters were set up to replicate Equations (12) and (31) such that;

|  |  |  |
| --- | --- | --- |
|  | . | (39) |

For the ODE to describe a moving pond,Equation (23), we used the inbuilt ODE equation ‘Global ODE’ to calculate. The ‘Global ODE’ takes the form:

|  |  |  |
| --- | --- | --- |
|  | . | (40) |

To write Equation (23) in this form, the ‘Global ODE’ is set up such that

|  |  |  |
| --- | --- | --- |
|  | , | (41) |

where

|  |  |  |
| --- | --- | --- |
|  |  | (42) |

and

|  |  |  |
| --- | --- | --- |
|  | . | (43) |

The integral in Equation (43) was calculated with the inbuilt ‘Boundary Integration Component Coupling’ by a summation over the nodes along the top domain boundary.

*Boundary conditions*

For the flux boundaries used, Equations (16), (25), (32), (33) and (34), we used the inbuilt flux boundary condition that takes the form,

|  |  |  |
| --- | --- | --- |
|  | , | (44) |

where and depend on the specific flux boundary. Similarly, for the constant boundary condition Equation (26), we used the inbuilt Dirichlet boundary condition. This takes the form:

|  |  |  |
| --- | --- | --- |
|  | , | (45) |

where the parameter value used is described in the parameters section.

For the constant hydrostatic boundary, Equation (19), we could not impose the generic inbuilt Dirichlet boundary condition because it treats the constant boundary as a step function such that

|  |  |  |
| --- | --- | --- |
|  | . | (46) |

This in turn leads to a permanent fully saturated boundary along the bare soil surface. To avoid this problem, we re-write Equation (19) as a flux condition along such that

|  |  |  |
| --- | --- | --- |
|  | , | (47) |

where . As increases, Equation (47) reduces to. Therefore, Equation (19) can be approximated and imposed as a flux condition along the partition only, providing is significantly large. We chose because this is sufficiently large to cause.

**Figure captions**

**Figure 1**Half of a ridge and furrow period, where is the total soil domain such that, is the region of soil with no roots, is the region of soil with roots present, is the soil surface boundary, is the base of the domain, is the left boundary adjacent to the ridge and is the right boundary adjacent to the furrow. The curve is generated from the values and used in the periodic function, Equation (1).

**Figure 2**Half of a ridge and furrow period, where is the soil surface boundary on which ponding occurs, is the soil surface that is not ponded, is the point on the soil surface where the pond begins, is the width of the half period of ridged domain, is the maximum depth of the pond, is the curve for the soil surface and is the volume of the pond.

**Figure 3**The heavy and light rainfall regimes used in the numerical simulations.

**Figure 4**Time series of saturation plots across the domain at various times before, during and after the first rain event described by the heavy rainfall regime and no plants. The first three plots (a)–(c) show the water profile before, during and at the end of the rainfall event, respectively, where represents the start of the 4-hour rain event. The last six plots (d)–(i) show the water profile after the rain event, where denotes the end of the rain event. The pond location is indicated by a black star along the surface curve of the geometry.

**Figure 5**Solute concentration profiles for a mobile solute (buffer power ) 16 weeks after solute application under the two rainfall regimes: (a) shows the results from the heavy rainfall regime (which causes ponding) without water uptake in the ridges of the geometry, (b) is the light rainfall regime without root uptake, (c) is the heavy rainfall regime with root uptake and (d) is the light rainfall regime with root uptake.

**Table 1**Parameter values for various soil types ([van Genuchten, 1980](#_ENREF_34)), where is the porosity of the soil, is the saturated hydraulic permeability, is the characterstic suction pressure and is van Genuchten parameter.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Soil type |  |  |  |  |
| Hygiene Sandstone | 0.250 |  | 12 400 | 0.9 |
| Silt Loam G.E.3 | 0.396 |  | 23 200 | 0.51 |
| Guelph Loam (Drying) | 0.520 |  |  8500 | 0.51 |
| Beit Netofa Clay | 0.446 |  | 64 500 | 0.15 |

**Table 2**Model parameter values used in numerical simulation.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Parameter | Description | Value | Units | Reference |
|  | Density of water |  |  |  |
|  | Acceleration due to gravity |  |  |  |
|  | Buffer power |  |  | ([Barber, 1995](#_ENREF_4)) |
|  | Diffusion coefficient in free liquid |  |  | ([Shackelford & Daniel, 1991](#_ENREF_28)) |
|  | Van Genuchten parameter |  |  | ([van Genuchten, 1980](#_ENREF_34))  |
|  | Porosity |  |  | ([van Genuchten, 1980](#_ENREF_34))  |
|  | Saturated water permeability |  |  | ([van Genuchten, 1980](#_ENREF_34)) |
|  | Characteristic soil suction |  |  | ([van Genuchten, 1980](#_ENREF_34)) |
|  | Impedance factor |  |  | ([Nye & Tinker, 1977](#_ENREF_21); [Roose & Fowler, 2004b](#_ENREF_25)) |
|  | Viscosity of water |  |  | ([Watson *et al.*, 1980](#_ENREF_37)) |
|  | Root surface area density water conductivity |  |  | ([Kirkham *et al.*, 1974](#_ENREF_13); [Lesczynski & Tanner, 1976](#_ENREF_15); [Rawsthorne & Brodie, 1986](#_ENREF_22); [Steudle *et al.*, 1987](#_ENREF_31); [Roose & Fowler, 2004a](#_ENREF_24)) |
|  | Root xylem pressure |  |  | ([Liu *et al.*, 2006](#_ENREF_17)) |
|  | Saturated – partially saturated interface |  |  |  |
|  | Minimum pond depth |  |  |  |
|  | Infiltration capacity |  |  | ([Morin & Benyamini, 1977](#_ENREF_18)) |
|  | Variation in soil depth |  |  | ([Steele *et al.*, 2006](#_ENREF_30); [Li *et al.*, 2007](#_ENREF_16)) |
|  | Ridge wave number |  |  | ([Steele *et al.*, 2006](#_ENREF_30); [Li *et al.*, 2007](#_ENREF_16)) |
|  | Average soil depth |  |  | ([Steele *et al.*, 2006](#_ENREF_30); [Li *et al.*, 2007](#_ENREF_16)) |
|  | Geometry width |  |  | ([Steele *et al.*, 2006](#_ENREF_30); [Li *et al.*, 2007](#_ENREF_16)) |