

Predicting infiltration pollutant retention in bioretention sustainable drainage systems: model development and validation

Ruth Quinn and Alejandro Dussailant

ABSTRACT

A major problem of increased urbanization is the rise in pollution caused by runoff. A solution to this problem can be found through the use of Sustainable Urban Drainage Systems (SUDS) such as rain gardens. Previous research has focused primarily on hydrologic design including the degree to which groundwater is replenished by these systems and models have been developed to quantify the extent of that recharge. However these models do not simulate the transport or fate of pollutants. In this paper, a preliminary heavy metal retention computer model is proposed that consists of two parts: a water flow module and pollutant retention module. To describe flow behaviour a dual-permeability approach is implemented which facilitates the prediction of both matrix and macropore flow. This subroutine is then combined with the retention module, which utilizes and couples the linear, Langmuir and Freundlich isotherms with the advection-diffusion equation. Both submodels are validated using existing literature data. This validation was assessed using efficiency indexes and showed good results with an $R^2 > 0.93$ for the matrix region, an $R^2 > 0.89$ for the macropore region and an $R^2 = 0.99$ for the pollutant retention module. This results in a valuable tool for the design and implementation of bioretention facilities.

Key words | dual-permeability model, heavy metals, rain garden, sustainable drainage

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INTRODUCTION

One of the major effects of increasing urbanization has been the detrimental impact it has had on water quality (Paul & Meyer 2001; Duh *et al.* 2008; Liu *et al.* 2009). Urban runoff has become a major source of pollutants and has grown to be a significant degrader of lakes, rivers and other waterways in the UK with 11% of the total pollution in Scottish rivers attributed to it (D'Arcy *et al.* 2005). It is also an increasing problem in the United States where urban runoff is second only to agriculture as a source of river pollution (Ellis & Mitchell 2006).

A recent approach to deal with this problem has been the use of Sustainable Drainage Systems (SUDS, or Best Management Practices as they are referred to in North America), such as rain gardens (Bitter & Bowers 1994; Dussailant 2012). The latter are also commonly used to

mitigate ground water depletion (Dussailant 2002), another consequence of increased urbanization. A rain garden is a vegetated depression that has been specifically designed to collect and infiltrate the storm water running off impervious areas such as car parks, roofs and pavements. They are usually shallow depressions (less than 20 cm in depth) and are typically 5–20% of the size of the impervious surface from which they receive storm water (Dussailant *et al.* 2005), with a layered soil profile consisting of an organic matter rich root zone and underlying storage/transmission zone usually consisting of sand and gravel. They have numerous advantages such as increased groundwater recharge (Dussailant *et al.* 2004), pollutant retention and have been shown by Muthanna *et al.* (2007) to reduce peak stormflow volume.

Currently, they are not as prevalent in the UK as in other countries such as the USA where guidelines have been in place since the 1990s to promote their use (PGC 1999; Wisconsin Department of Natural Resources 2012). However their popularity in England and Wales is certain to increase with the introduction of legislation such as the Flood and Water Management Act (2010), which promotes the use of SUDS in new developments and redevelopments by requiring drainage systems to be approved against a set of National Standards (Department for Environment Food and Rural Affairs 2011). Because of this and the growing pollution caused by urban runoff, research into the design and performance of these facilities is of increasing importance.

Previous research has been completed on water balance design and into the degree to which groundwater is replenished by these systems and computer models have been developed to quantify and optimize the extent of that recharge: models RECHARGE (Dussaillant *et al.* 2004); RECARGA (Dussaillant *et al.* 2005) and R2D (Aravena & Dussaillant 2009). However these models do not simulate pollutant loading and removal. The ability of a rain garden to retain pollutants has been proven through various laboratory experiments and field monitoring (Hsieh & Davis 2005; Li & Davis 2008a; Hatt *et al.* 2009). It was found by Hatt *et al.* (2009) that over 91% of copper (Cu), lead (Pb) and zinc (Zn) were removed by a rain garden in McDowell Australia. However previously there has been no method to continually simulate this retention based on the changeable hydrological and material factors on which it is dependent. Thus, a simple design tool is needed which has the ability to estimate the extent to which contaminants are retained in a given bioretention facility. As performed by water-design models mentioned previously, this model could be used to inform design by running with long-term fine-resolution data (e.g. 30 years of hourly rainfall), climate change scenarios, varying pollutant loading and different soil layer types, to optimize the facilities in terms of design parameters.

An important factor that has been seen to impact the retention of pollutants is preferential flow from macropores. These are large continuous openings in soil, which can result in the rapid downward movement of solutes and pollutants through the soil system (Beven & Germann

1982). Pollutant retention is predominately seen in either the upper layers of the system or through vegetation uptake (Hong *et al.* 2006; Sun & Davis 2007; LeFevre *et al.* 2012). The transport of the runoff rapidly through the system via macropores would bypass both these mechanisms and could result in ground water contamination. There are several types of macropore that have been identified, formed by soil fauna (i.e. earthworms), by plant roots, cracks and fissures and natural soil pipes (Beven & Germann 1982). To the authors' knowledge, no research has been completed into macropore formation specifically in rain gardens. However bioretention systems will develop macropores during their lifecycle owing to bioturbation, plant root and soil fauna (e.g. earthworms). Thus in order to accurately quantify the retention of pollutants in a bioretention system, it is necessary to take this form of preferential flow into account.

The aim of this paper is to present a user-friendly model with few and easily obtainable parameters to ensure widespread use. Current water transport pollution models, such as HYDRUS (Simunek *et al.* 2009), MACRO (Larsbo & Jarvis 2003) and RZWQM (Ahuja *et al.* 2000), are not appropriate for this task for a variety of reasons. Firstly, they are primarily used for agrochemicals and thus would have to be significantly adapted to include important urban stormwater pollutants such as heavy metals. Secondly, most of these models are based on the Richards equation (used by both HYDRUS and MACRO), which would impair long-term detailed modelling for design purposes due to the processing times required for a detailed simulation of a dynamic layered system such as a bioretention cell (Larsbo & Jarvis 2003; Simunek *et al.* 2009). Finally these models require a large amount of expertise, training and input parameters which may prevent widespread use. To date, guidance on the numerical prediction of pollutant retention in actual SUDS facilities where phenomena such as macropore flow exists is lacking. A dual permeability (matrix and macropore flow) model considering heavy metal retention is presented which meets the requirements stated above.

To design such a complex model it was decided to initially focus on one element of the runoff pollution; this was chosen to be heavy metals for a variety of reasons. Metals can accumulate in the upper layers of the system and pose a significant health hazard unlike nutrients or

hydrocarbons that biodegrade or are taken up by vegetation more easily (Hong *et al.* 2006; Sun & Davis 2007; LeFevre *et al.* 2012). Regulatory guidelines for heavy metals in residential soil exist in the US and are based on child exposure to soil at home or other corresponding locations (Petersen *et al.* 2006) and it has been shown that levels of Pb in the upper layers of a rain garden can exceed these limits (Li & Davis 2008a). Rain gardens are not necessarily situated in residential areas; however they may be accessible to children thus potentially causing a health hazard. In addition the isotherms which have been preliminarily suggested for heavy metal sorption can also be used to model sorption of nutrients and hydrocarbons allowing for the inclusion of these pollutants in this model at a later date (Hong *et al.* 2006; Langergraber & Simunek 2006; Li & Davis 2008b). Finally all the above contaminants depend on water modelling factors such as macropore flow (Beven & Germann 1982). The proposed model will predict these factors independent of heavy metal retention. This allows for the addition of subroutines in the future which can predict other phenomena (e.g. nutrient uptake).

The specific objectives for this paper were:

1. to create a model that accounts for the effects of matrix and macropore flow and considers pollutant retention, initially applicable for metals;
2. to validate the model in terms of both water flow and the ability to retain the pollutants and also the degree of pollutant build-up in the system.

By meeting these objectives, this computer model will provide a valuable tool for the design and implementation of bioretention facilities.

METHODS

Heavy metal retention modelling

A number of studies have been completed into heavy metal concentrations in urban runoff and it has been found that the levels are highly variable and location dependent (Gromaire *et al.* 1999; Turer *et al.* 2001; Gobel *et al.* 2007). Gobel *et al.* (2007) identified that a residential neighbourhood's levels of Cu are higher than in heavily trafficked areas owing to

its use in roof construction. However they found that on roads, levels of cadmium (Cd), chromium (Cr), Pb and Zn were substantially greater than in these residential areas.

It has been found in the majority of cases for rain garden systems that heavy metals have been almost completely removed despite the variability in their concentrations. The vast majority of this removal occurs in the first 25 cm of soil (Sun & Davis 2007; Li & Davis 2008a). Adsorption has been identified as the dominant heavy metal removal mechanism accounting for over 88% of the total removal with the remainder either accumulated by plants (0.5–3.3%) or not captured (Sun & Davis 2007). From this information it is clear that the process of adsorption is by far the most important mechanism by which heavy metals are removed. The use of isotherms has proven to be the most effective method of predicting the sorption of metal ions onto soil in the past (Ho *et al.* 2002; Jang *et al.* 2005; Sun & Davis 2007). Though there are many isotherms equations in existence, the linear and Langmuir have previously proved most effective, accurate and convenient for modelling heavy metal adsorption (Jang *et al.* 2005; Li & Davis 2008a).

The linear isotherm is the simplest: it assumes that the media-sorbed pollutant concentration (C_s) is directly proportional to the dissolved pollutant concentration (C)

$$C_s = K_d C \quad (1)$$

where K_d is the distribution coefficient. The distribution coefficient is one of the determining factors of pollutant retention; it is a measure of the ability of a medium such as soil to retain contaminants and varies between both media and metals. Li & Davis (2008a, b) modelled the absorption of Cu, Pb and Zn in a rain garden using a linear isotherm. Their results indicate a successful prediction of heavy metal retention especially in the cases of Pb and Zn. The retention of Cu however was not modelled as accurately, possibly owing to its weaker association with the soil, desorption or incorrect linear assumptions. Li & Davis (2008a, b) concede that if a more accurate numerical model is required, non-steady state and nonlinear isotherms would be needed but this would increase model complexity and input data requirements. Therefore the Langmuir isotherm is also incorporated into this model, as it has previously proved effective at modelling heavy metals (Jang *et al.* 2005). However, the linear isotherm is the most

convenient to use as it requires the fewest parameters; it is thus the primary isotherm included. Other isotherms (Langmuir and Freundlich) can be used if their parameters are available.

The Langmuir isotherm has conventionally been used to assess and compare the capacities of various bio-sorbents. At low pollutant input concentration levels, it essentially reduces to a linear isotherm; at higher concentrations it assumes monolayer adsorption (Foo & Hameed 2010). The nonlinear form of the Langmuir isotherm can be represented as follows:

$$C_s = \frac{K_L S_{\max} C}{1 + K_L C} \quad (2)$$

where K_L is the Langmuir isotherm constant and S_{\max} is the total concentration of sorption sites available.

The Freundlich isotherm can be used in situations where the Langmuir isotherm is inappropriate such as for coarse-grained soils. This is useful as typically the lower drainage layers of rain gardens consist of granular material such as sand. Additionally, pH can be easily integrated into the Freundlich isotherm, to be discussed later. It is an empirical model which can predict non-ideal sorption as well as multi-layer sorption and has been extensively applied in heterogeneous systems (Ho *et al.* 2002)

$$C_s = K_F C^{a^F} \quad (3)$$

where K_F is the Freundlich constant and a^F is the Freundlich exponent.

To incorporate adsorption with the transport aspect of the pollutant modelling the following adsorption advection diffusion equation developed by Ogata & Banks (1961) is proposed:

$$C_s(x, t) = \left(\frac{C}{2}\right) \times \left\{ \operatorname{erfc} \left[\frac{(Rx - vt)}{2\sqrt{RDt}} \right] + \exp\left(\frac{vx}{D}\right) \operatorname{erfc} \left[\frac{(Rx + vt)}{2\sqrt{RDt}} \right] \right\} \quad (4)$$

where x and t are the positions in space and time, respectively, erfc is the complementary error function, v is the pore water velocity, D is the diffusion coefficient, R is the retardation factor which governs the retention of the pollutants and is dependent on the isotherm being used.

The value of R can be calculated for the selected isotherms as presented in Table 1 where θ is the soil moisture content.

The use of these retardation coefficients allows for the prediction of retention as a function of both the depth of the system (which enables examinations regarding the maximum depth to which contaminants travel in the rain garden) and the time (which allows for quantification of the metal concentrations accumulating in the system).

An additional contributor to the retention of heavy metals in a rain garden system not taken into account by these isotherms is suspended solids, identified by Li & Davis (2008a, b). The metals in urban runoff can easily sorb to these solids and be removed in the rain garden through the process of filtration. This can lead to clogging of the system which is addressed by Jenkins *et al.* (2010). However when examined in greater detail it was found that these solids have a negligible impact on heavy metal capture, accounting for less than 1% of the retention and so are not included in this model (Li & Davis 2008a, b).

Another crucial factor affecting heavy metal retention is soil pH which affects the metal-solution and soil-surface chemistry and thus adsorption. Usually, heavy metal adsorption is small at low pH values as the quantity of negatively charged surface sites is low and increases with pH. Adsorption then increases at intermediate pH values from near zero to near complete adsorption over a small pH range; known as the pH-adsorption edge. At high pH values, heavy metals are completely removed from the runoff. This result has been shown by both the findings of Bradl (2004) and Christensen *et al.* (1996) who observed that the adsorption capacities of soils for metals decreased with pH.

As pH has such an impact on adsorption, it has been attempted to quantify its effects using an extension of the

Table 1 | Retardation coefficients for isotherms

Isotherm	Retardation factor (R)
Linear	$R = 1 + \frac{\rho}{\theta} K_d$ (5a)
Langmuir	$R = 1 + \frac{\rho}{\theta} \frac{K_L S_{\max}}{(1 + K_L C)^2}$ (5b)
Freundlich	$R = 1 + \frac{\rho}{\theta} (a^F K_F C^{a^F - 1})$ (5c)

Freundlich isotherm: van der Zee & van Riemsdijk (1987) thus suggested the inclusion of soil pH and organic carbon oc (measured as percentage by weight) in the Freundlich isotherm

$$C_s = k_f(H^+)^a oc^b C^M \quad (6)$$

where k_f is the Freundlich constant with dependencies on organic carbon and hydrogen activity H^+ eliminated and a_f , b_f and M_f are equation parameters which require calibration. This results in a retardation factor for the Freundlich isotherm of

$$R = 1 + \frac{\rho}{\theta} \left(M_f (H^+)^{a_f} oc^{b_f} k_f C^{M_f - 1} \right) \quad (7)$$

This equation accurately reflects the molecular impact pH has on heavy metal retention and would be useful as a tool for assessing metal capture across the pH range from extremely acidic to basic soils. However as can be seen, as well as increasing accuracy it also brings additional complexity. As a rain garden is an artificial creation, it is possible to use soils in the optimum pH range; the pH of the soil can then be maintained. Of course this approach is not appropriate in areas that are prone to acid rain but it is possible to assess these cases separately. Thus this equation is built into the model so that if these parameters are known the effect of pH on retention can be predicted.

Matrix and macropore modelling

It is clear from the review above that the most important hydrological factors for the retention of pollutants are velocity, diffusivity and water content. In order to quantify these effectively a dual permeability model is proposed for the modelling of water flow (Larsbo & Jarvis 2003; Simunek *et al.* 2009). The ability of any hydraulic model to predict both matrix and macropore flow is crucial in layered bioretention facilities as macropore flow can cause the contaminated water to bypass the adsorptive upper layer and be transferred into the lower infiltration layer where retention is less likely. There are three key factors to be considered in all dual permeability models: the initiation of

macropore flow, infiltration into both macropore and matrix regions and interaction between them.

Initiation of macropore flow

Initiation of macropore flow is a complex process often not accurately quantified by current dual permeability models (Nimmo 2012). Models such as MACRO, RZWQM and IN³M often use predefined values for saturation in the matrix region to determine the point at which macropore flow begins (Ahuja *et al.* 2000; Larsbo & Jarvis 2003; Weiler 2005). However this assumption has not been verified by experimental and field results and observations. It has been shown that macropore flow can take place in a variety of different scenarios not taken into consideration by previous models such as in soil much drier than saturation. An additional significant finding was that higher moisture contents can actually reduce macropore flow (Nimmo 2012).

The models above were designed for agricultural purposes; however rain gardens experience significantly more water input per unit area than agricultural conditions as they receive runoff from the impervious surfaces surrounding them (Dussaillant *et al.* 2004, 2005). This sudden increase in infiltration rates especially after prolonged dryness would most probably result in macropore flow as shown by Pot *et al.* (2005). They observed that in grass filter strips macropore flow occurred before saturation during high intensity events. This circumstance can occur in rain garden facilities and as such needs to be taken into account by the model.

In addition during prolonged periods of relatively light rainfall or in circumstances when the ground is already saturated, ponding occurs, which activates macropore flow. In these conditions it may be more apt to utilize the saturated switching point proposed by the RZWQM and IN³M (Ahuja *et al.* 2000; Weiler 2005). Therefore a dual equation plan is proposed for this model whereby for periods of prolonged low intensity rainfall, matrix flow would dominate until the point of saturation whereby macropore flow would occur. When water input occurs especially after dry periods (in which fissures and cracks may be present in the soil which exacerbate preferential flow), macropore flow would take place automatically. This pattern is further validated by the findings of Weiler & Naef (2005) who

examined the initiation of surface and subsurface macropore flow. For the purpose of this model, subsurface initiation is not considered as it has been shown that this form of initiation occurs predominantly in the lower half of the soil profile, commonly below 50 cm (Weiler & Naef 2005).

This should only minimally affect the soil pollution retention capacity as it has been shown that heavy metals are removed in the top 10 cm of soil (Sun & Davis 2007). It also has not previously been accounted for in other dual-permeability models such as MACRO and HYDRUS as it is difficult to quantify and does not significantly affect pollutant retention (Larsbo & Jarvis 2003; Simunek *et al.* 2009). Thus in this model, subsurface initiation of macropore flow will be neglected.

Infiltration

After examining several of the most common and well-used existing dual permeability models (RZWQM, HYDRUS, MACRO, IN³M), it was decided that both the matrix and macropore regions will be modelled using the kinematic wave equation (KWE) presented in one form as

$$\frac{\partial h}{\partial t} + v \frac{\partial h}{\partial x} = 0 \quad (8)$$

where h is the soil water head.

This method has proved successful previously at modelling water in the matrix region for situations that would be prevalent in a rain garden system such as complex surface flux patterns and layered soil (Smith 1983). Its accuracy has also been shown at replicating flow in macropores and being applied by widely used computer models such as MACRO (Larsbo & Jarvis 2003). By using this approach, the flow in both regions can be predicted using the same method. This meets the objective set of producing a simple design tool, over a more complex approach such as the Richards equation. It also allows for long-term modelling utilizing, for example, decades of hourly data, or several climate change scenarios. It also facilitates detailed testing of the effects of different parameter values such as different soil types and soil layer depths.

The pore water velocity is also of crucial importance to pollutant retention. For a leading wave, generated by a flux

q_u with θ increasing from θ_i to θ_u across the wave, the shock wave velocity can be represented as (Smith 1983)

$$v = \frac{q_u - q_i}{\theta_u - \theta_i} \quad (9)$$

where the flux q can be obtained from a transformation of the Richards equation that includes diffusivity, D (Smith 1983)

$$q = -D(\theta) \frac{d\theta}{dx} + K(\theta) \quad (10)$$

However, for a simple wetting front advance case this can be further simplified, as $\partial\theta/\partial x$ is negligible, $q(\theta)$ is simply $K(\theta)$ and the velocity equation becomes (Smith 1983)

$$v = \frac{K(\theta_1) - K(\theta_2)}{(\theta_1 - \theta_2)} \quad (11)$$

The soil moisture content can be calculated using van Genuchten–Mualem equations (Mualem 1976; van Genuchten 1980), assuming there is no hysteresis

$$\theta(h) = \frac{\theta_{\text{sat}} - \theta_{\text{res}}}{[1 + (\alpha|h|)^n]^m} + \theta_{\text{res}} \quad (12)$$

where θ_{sat} is the saturated soil water moisture content, θ_{res} is the residual soil water content, α is the van Genuchten parameter, n is the van Genuchten parameter (with $n > 1$) and $m = 1 - 1/n$.

For the macropore region velocity is given as (Mdaghri-Alaoui & Germann 1998)

$$v = \frac{dq}{dz} = abw^{(a-1)} = ab^{1/a}q^{(a-1)/a} \quad (13)$$

where w is the fraction of moisture content which contributes to the rapid flow, b is the hydraulic conductance and a is a dimensionless exponent which can indicate the flow regime (i.e. $a = 2$ for fully macropore flow and $a > 11$ for non-macropore flow).

Interaction between regions

To model the interaction between the soil matrix and macropore regions, a simple method detailed in the dual-permeability model proposed by Weiler (2005) is used,

whereby water movement only occurs in the macropore to matrix direction and the inflow into one macropore (q_{int}) is represented by the following equation:

$$q_{\text{int}}(t) = \pi \left[y(t)^2 - y(t - \Delta t)^2 \right] \frac{\Delta x \Delta \theta}{\Delta t} \quad (14)$$

where $y(t)$ is the lateral distribution of the wetting front at time t and $y(t - \Delta t)$ is the radial distance of the wetting front at the previous time. The assumption of flow solely in the direction of macropore to matrix region is present in other dual-permeability models such as RZWQM (Ahuja *et al.* 2000). The above equation was chosen since it needs fewer parameters than methods that require retention curves for both water flow regions (Larsbo & Jarvis 2003; Simunek *et al.* 2009).

The model was validated using published literature results which involved conditions prominent in rain garden facilities, specifically layered soil profiles and sharp wetting fronts. In order to determine the accuracy of the model several efficiency indexes were used to evaluate the goodness-of-fit. These were: the coefficient of determination (R^2), the Nash-Sutcliffe coefficient and the root mean square error. Each of these indexes gives specific information regarding the precision of the model so by utilizing them all an overall picture of its accuracy can be gathered. The coefficient of determination provides an estimate of the proportion of overlapping variance between the experimental and model result. This result may contain biases, however, which are taken into account by the Nash-Sutcliffe coefficient which has shown great utility in hydrologic research being used to evaluate model simulations of discharge, and water quality constituents such as sediment, nitrogen, and phosphorus loadings (McCuen *et al.* 2006). Finally the root mean square error is a measure of the average distance of an experimental result from the model simulation, measured along a vertical line; as it is directly interpretable in terms of measurable units, it can offer additional information to that of other correlation coefficients.

RESULTS

To facilitate the identification of any faults with the various components of the model, it was split into three parts:

matrix, macropore and pollutant retention for ease of validation.

Part 1: Matrix region

The validation of this region comprised testing the model against two differing scenarios. The first was a 24 hour simulation of sharp wetting front carried out by Celia *et al.* (1990), where the soil column was 100 cm deep, $\theta_{\text{sat}} = 0.268$, $\theta_{\text{res}} = 0.102$, $K_{\text{sat}} = 33.2 \text{ cm h}^{-1}$, $\alpha = 0.0355$, $n = 2$, homogeneous initial head distribution of $-1,000 \text{ cm}$, and the upper boundary condition is fixed at -75 cm . The velocity of the kinematic wetting wave was calculated using Equation (11) and found to be 2.4 cm h^{-1} . The model results agree well with those of Celia *et al.* (1990) as can be seen in Figure 1.

Along with a visual agreement, the efficiency indexes also showed good results which are given in Table 2.

As is illustrated by Figure 1 the main source of error occurs at the onset of the sharp wetting front owing to a minor numerical instability; however despite this it is clear that the kinematic wave equation still exhibits satisfactory results.

The second validation case was chosen to be the layered soil profile case 1.2 of Pan & Wierenga (1995); the soil characteristics are given in Table 3. The velocity of the sharp wetting front was calculated using Equation (11) and found to be 4.2 cm h^{-1} in the upper layer.

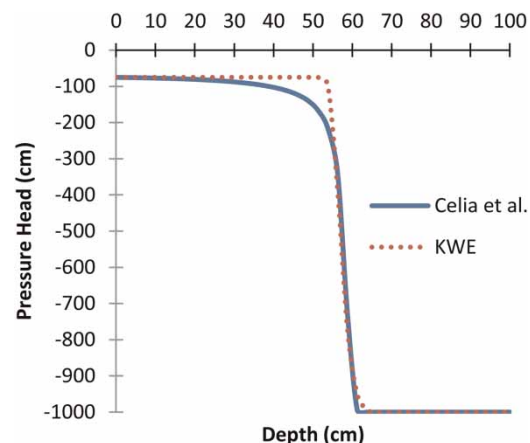


Figure 1 | Comparison of KWE results with Celia *et al.* (1990) model.

Table 2 | Efficiency indexes for the model and Celia *et al.* (1990) results

Error estimator	Result
Coefficient of determination	0.996
Nash-Sutcliffe efficiency index	0.995
Root square mean error (cm)	30.5

The initial condition is suction head profile of $-1,000$ cm, the upper boundary condition is a constant rainfall rate of 1.25 cm h^{-1} and the lower boundary condition is zero flux. The model yields similar results for both pressure head and soil volumetric water content predictions as seen in Figures 2(a) and 2(c). A comparison is also shown between KWE and RECHARGE (Dussailant *et al.* 2004) to illustrate a comparison between the results of a complex equation such as Richards (which RECHARGE uses) and the simpler KWE.

Efficiency indexes were calculated for the above simulations and are listed in Table 4.

Again, the main source of error occurs at the onset of the sharp wetting front (Figures 1 and 2), though from Table 4, a good correlation is still seen.

The results of these validation runs illustrate that this model can successfully handle the situations of sharp wetting fronts, dry initial conditions and layered soil profiles in the matrix region, conditions common to rain gardens. It was therefore decided to continue to validate the model for the macropore flow case.

Part 2: Macropore region flow

The movement of flow through the macropore is one of the most crucial aspects in relation to pollutant modelling as it

quantifies the total volume of water through the pores and also the velocity of this movement. Thus the following column experiments completed by Mdaghri-Alaoui & Germann (1998) were chosen as suitable validation cases for the macropore segment of this model as the six runs which were performed on a layered soil encompass a range of infiltration, conductance and exponent values. Runs 3–6 are shown here and their soil characteristics are shown in Table 5.

The kinematic wave velocity, v as shown in Table 5 was calculated using Equation (13). Mdaghri-Alaoui & Germann (1998) undertook these experiments to examine the drainage outflow for several infiltration rates, on soil which originated from calcareous silty-sandy lake sediments. The upper layer 0–0.16 m was well structured with a porosity of 0.52 and a sandy loam texture, the lower layer below 0.16 m had a porosity of 0.5 and was sandy in consistency. The bulk density was found to increase slightly with depth.

A comparison between the KWE prediction and the experimental results for cases 3–6 is shown in Figure 3.

The model accurately captures the peak flow rate (Figure 3) but fails to fully predict the drainage wave in cases 3 and 4, yet at higher input rates the correlation between the experimental and model drainage wave improves (cases 5 and 6). Despite these slight inaccuracies the R^2 value is still high (Table 6) with values of over 0.89 in all cases.

Part 3: Pollutant retention

The linear isotherm method was validated against the experimental results of Davis *et al.* (2001). This dataset was chosen as the experiments were specifically focused on bioretention

Table 3 | Mualem-van Genuchten parameters of Pan & Wierenga (1995) Case 1.2

Soil characteristic	Top layer	Middle layer	Lower layer
Texture	Loamy fine sand	Clay loam	Loamy fine sand
Depth (cm)	10	30	10
α (cm^{-1})	0.028	0.010	0.028
n	2.24	1.4	2.24
θ_{res} ($\text{m}^3 \text{ m}^{-3}$)	0.0286	0.106	0.0286
θ_{sat} ($\text{m}^3 \text{ m}^{-3}$)	0.366	0.469	0.366
K_{sat} (cm h^{-1})	22.5	0.546	22.5

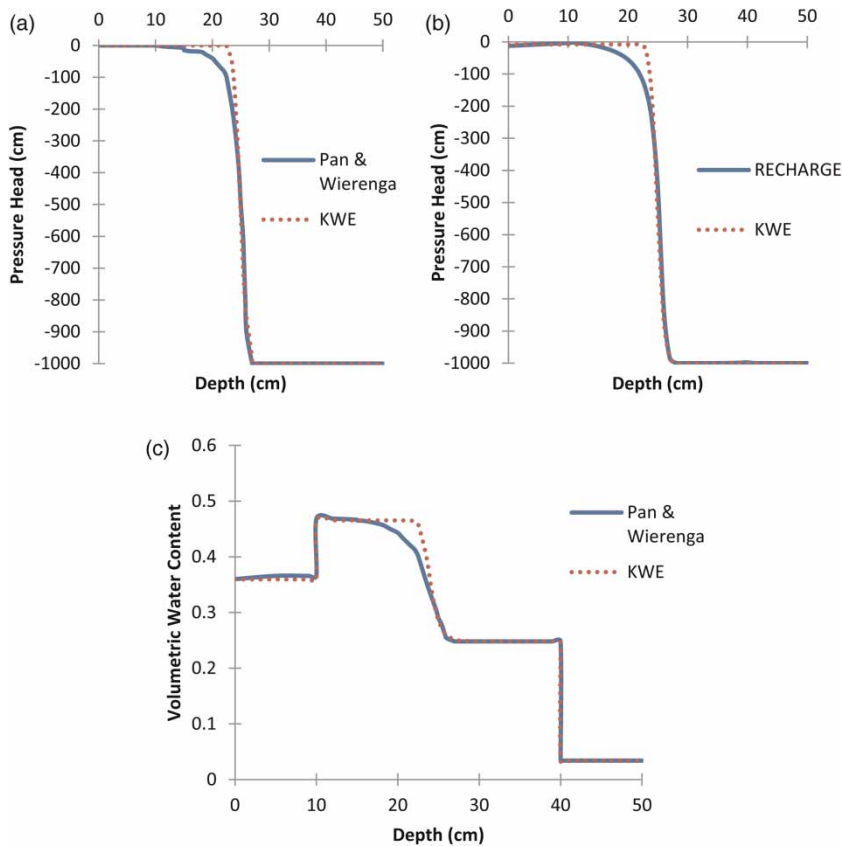


Figure 2 | Comparison of the results from the model with layered soil simulation with case 1.2 of Pan & Wierenga (1995): (a) pressure head simulation KWE, (b) pressure head simulation KWE and Pan & Weirenga RECHARGE, (c) soil moisture content.

Table 4 | Efficiency indexes for the model and case 1.2 of Pan & Wierenga (1995)

Efficiency index	Pressure head	Volumetric water content
Coefficient of determination (r^2)	0.993	0.931
Nash-Sutcliffe efficiency index	0.990	0.921
Root square mean error	43.6 cm	0.0380 m ³ m ⁻³

performance. They consisted of the heavy metal retention evaluation of several small columns (3.5 cm depth) filled with topsoil (parameters shown in Table 7).

Figure 4 shows the total concentration of Cu absorbed by the soil. It is clear from this figure that an accurate correlation between experimental and model results is seen, with only a small divergence in results after approximately 10 hours. However, despite this small inaccuracy, the

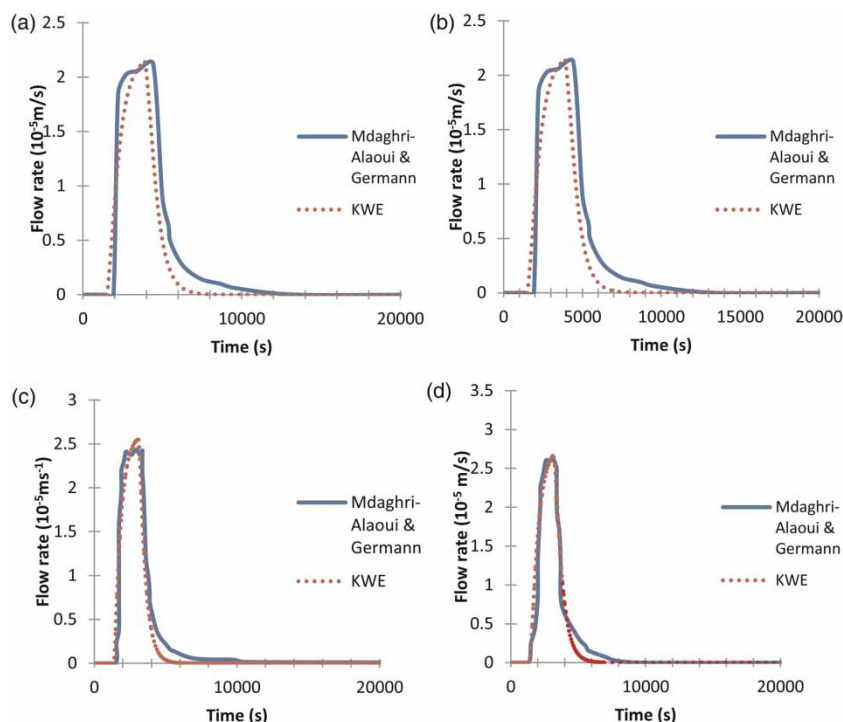
efficiency indexes for this simulation (shown in Table 8) display a good agreement between model and experimental data.

DISCUSSION

In summary, results for the hydrological segment of the model correlate well with the chosen literature cases with an R^2 of over 0.93 (for matrix flow) and 0.89 (for macropore flow). Some minor discrepancies are found between the model simulation and experimental results for the macropore drainage flow possibly owing to the occurrence of some matrix flow, which would lead to a gentler drainage curve. This is supported by the value of the parameter a which for the experiments ranged from 4.38 to 5.6 indicating transitional flow tending towards macropore as opposed to pure preferential flow (which has a value of $a = 2$). Despite

Table 5 | Parameters from Mdaghri-Alaoui & Germann (1998)

Parameter	Case 3	Case 4	Case 5	Case 6
Total soil depth (cm)	43			
Column diameter (cm)	39			
Upper boundary condition q_s (cm)	7.92	8.28	9.4	10.1
Duration of infiltration (s)	4100	4500	4000	3000
A	4.77	4.73	4.38	5.60
b (cm h ⁻¹)	1.52 × 10 ⁶	1.63 × 10 ⁶	0.69 × 10 ⁶	15.3 × 10 ⁶
Velocity v (cm h ⁻¹)	102	109	122	128

**Figure 3** | Comparison of KWE with run 3 in Mdaghri-Alaoui & Germann (1998): (a) case 3, (b) case 4, (c) case 5, (d) case 6.**Table 6** | Efficiency indices for the model and cases 3–6 of Mdaghri-Alaoui & Germann (1998)

Efficiency index	Case 3	Case 4	Case 5	Case 6
Coefficient of determination	0.93	0.92	0.89	0.96
Nash-Sutcliffe efficiency index	0.80	0.90	0.87	0.96
Root square mean error (×10 ⁻⁵ m s ⁻¹)	0.386	0.253	0.330	0.204

Table 7 | Parameters from Davis *et al.* (2001)

Parameter	Value
Copper input concentration (µg L ⁻¹)	90
Depth of column (cm)	3.5
Diameter of column (cm)	1.9
Input rate (cm h ⁻¹)	63.6
Duration of input (hours)	50
Bed volume (cm ³)	9.9
Linear adsorption coeff. (L Kg ⁻¹)	550

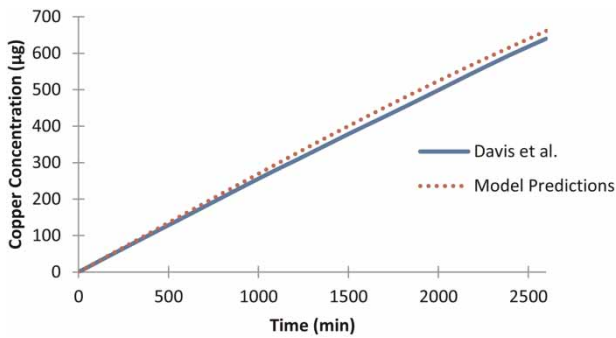


Figure 4 | Comparison of model results for Cu retention with experiments of Davis *et al.* (2001).

Table 8 | Efficiency indexes for the model and Davis *et al.* (2001) results for Cu concentration

Error estimator	Result
Coefficient of determination	0.999
Nash-Sutcliffe efficiency index	0.993
Root square mean error (µg)	16.0

this, good prediction of macropore flow is still obtained especially at higher input rates, which are essential when modelling SUDS facilities, which receive large amounts of runoff from impervious surfaces, such as rain gardens. The hydraulic algorithm thus provided a suitable foundation for the overall model. The pollutant retention submodel also performed well in terms of its ability to predict pollutant build up in a system, with an R^2 of 0.999 and thus was deemed to be promising for replicating pollutant retention in a rain garden.

There are few models that predict heavy metal retention. Attempts have been made to create subroutines in HYDRUS to predict the heavy metal transport through soil. However this model was primarily aimed at investigating the leaching of highly mobile metals through minimally retentive soil and thus retention prediction was not a key feature (Simunek *et al.* 2009). As such, the model proposed by this paper is unique in its ability to predict retention in a SUDS facility and thus can be used as both a design tool and a method of appraising current facilities.

Additional heavy metal dynamics as a function of depth can be combined with the pollutant loading entering the system to provide a measure of the heavy metal build up

in the upper layers of the system. This can be used as an indication as to when this upper layer would need to be replaced. This is especially important, as levels of Pb in the upper layers of soil have been known to exceed safety guidelines in rain gardens (Li & Davis 2008a).

Finally, the simple equations used in the model also enable long-term simulations to be run in a relatively short amount of time. This would not be possible on existing dual-permeability models such as MACRO and HYDRUS as due to their complexities their computational times are far longer. Also as these models are not specifically designed for bioretention facilities, it would take specialist knowledge and a large degree of familiarity and investigation of parameters to utilize them as pollutant retention models for SUDS. As such, the model proposed in this paper is a far superior alternative to both these options and the minor inaccuracies it experiences when compared with other hydrological models which utilize the Richards equation (as illustrated by the comparisons in this paper) are more than compensated for by its utility.

CONCLUSIONS

The main aim of this paper was to develop and validate a computer model able to predict the extent to which heavy metals are retained in SUDS, such as rain garden bioretention systems based on both hydrological and design factors. In order to achieve maximum use, the main requirements of the model were established as simplicity, ease of use, only requiring few parameters to be estimated and as physically based as possible.

The proposed model consists of two parts: a water flow module and pollutant retention module. To describe flow behaviour a dual-permeability approach is proposed which will facilitate the prediction of not only matrix but also of macropore flow, which is considered key in bioretention systems consisting of vegetated soil due to bioturbation by roots and soil macrofauna. This module is then combined with the pollutant retention module, which utilizes isotherms previously proven accurate in heavy metal retention models and couples them with the advection-diffusion equation, which can both predict heavy metal capture and measure its accumulation.

The requirement of simplicity was fulfilled by utilizing relatively simple equations to describe the key aspects of dual-permeability flow: the KWE for macropore and matrix flow, a saturation and high intensity approach for macropore initiation and finally a simple equation to describe interaction between the regimes. The use of simple isotherms also limits the number of parameters needed for a sufficiently accurate estimate of retention.

The model was tested against literature data for matrix flow, macropore flow and heavy metal retention and was found to exhibit satisfactory results illustrated in terms of both a visual agreement of trends and various efficiency indexes. A minor divergence was detected for the pollutant retention validation, this was attributed to macropore flow occurring in the experiment which was not sufficiently measured and thus could not be quantified by the model. The model is ready for use but will be further validated using column experiments that will monitor hydrologic and water quality variables in a layered setup with preferential flow.

This model offers many advantages over manuals and guidebooks often used in SUDS design as individual bioretention facilities can be specifically evaluated. The simple equations used in the model also enable long-term simulations to be run in a relatively short amount of time which would not be possible with more complex models. It complements existing SUDS design models which did not include pollutant modelling and is applicable not only to rain gardens but other bioretention facilities as well. It thus serves as an additional tool, available to urban planners and engineers involved in the design, construction and evaluation of SUDS in urban environments.

ACKNOWLEDGEMENTS

This work was funded by the University of Greenwich RAE-11 grant and School of Engineering funding for PhD studentship.

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First received 14 September 2012; accepted in revised form 22 January 2014. Available online 14 February 2014