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"Chaos is the law of nature; order is the dream of man." Henry Adams (1918)

Abstract

We often develop models of the internal processes of buffer zones to predict the water-quality abatement potential associated with buffer zones of varying width, location and site characteristics. We also create models to illuminate our understanding of the interactions of water-quality contaminants with the biotic and abiotic factors within a buffer zone. In this paper, we explore a variety of models that simulate the fate of water-quality contaminants in buffer zones. Because of the central nature of hydrology to water-quality functions of buffer zones, we focus on the hydrologic components of buffer-zone models with special attention to the site-specific conditions that affect the flow path, residence time and soil environment encountered by water quality contaminants within a buffer zone. Throughout the paper, we address the effects of varying levels of spatial resolution on the ability of models to capture the site-specific processes inherent in buffer zones.

Application of the appropriate removal processes to waterborne contaminants requires estimates of flow paths and retention times within different portions of a buffer zone. Models can simulate the potential for contaminants to infiltrate into the soil or enter the buffer zone by subsurface flow. Once within the soil, methods exist to simulate a host of removal mechanisms including filtration, microbial transformations, plant uptake and adsorption. Modellers have also addressed situations where waterborne contaminants within the soil bypass rootzone process. For example, contaminated groundwater from the upland may travel below the biologically active portions of the soil or it may emerge at surface seeps and travel overland across the buffer zone. In addition, where preferential and macropore flow is likely, models can be constructed to reduce the expected groundwater residence time and related transformations.

Considerable information on buffer-zone processes can be inferred from conceptual or qualitative models that rely on spatial data, such as hydrogeomorphic setting, vegetation type, slope and the soil classification. Site-specific soil data such as texture, structure and depth to redoximorphic features will refine these models. Through the use of pedotransfer functions, these same data can serve to initialize more quantitative models that require information on soil moisture characteristic curves and hydraulic conductivity. Clearly, more mechanistic modelling approaches should require more explicit spatial and temporal inputs. In this paper, we review various methods used to simulate infiltration, the extent of saturation within the rootzone and groundwater seepage. In theory, to simulate these processes requires linkage to hillslope hydrologic factors – such as incoming flow rates and the relative elevation of the downgradient receiving water. These external hydrologic characteristics are highly dynamic, and models exist that incorporate the effects of daily fluctuations of external factors. However, given the seasonality of overland runoff and groundwater flow, useful insights may be obtained from static simulations representing the expected conditions within hydrologically active periods of the year.

INTRODUCTION

Vegetated buffer zones hold great promise for protecting streams and ponds from contaminated runoff and groundwater leaving upland areas. Because the performance of buffers is somewhat site-specific, there is great interest in new approaches to evaluate the water-quality functions of vegetated buffers. In this chapter, we describe models that focus on internal processes in buffers.

Why model internal processes? We recognize that field work is essential to any assessment of the water-quality functions of buffer zones. However, models provide us with the unique opportunity to study combinations of conditions which have not yet been encountered in field studies. With models, we can step back and gain a broader view with the purpose of detecting common patterns among sets of climatic and landscape conditions. This type of exercise would be difficult if we restricted ourselves to field data alone. Models of internal processes in riparian zones can also augment the development of qualitative management models. For example, models could be employed to evaluate and modify classification schemes that rank the potential capability of riparian zones to perform various water quality functions based on combinations of landscape, geology and land cover (Pinay and Décamps, 1988; Lowrance, 1997).

Models of water-quality functions in buffer zones encompass a wide range of approaches and complexity, arising mainly from the variety of the intended use and audience of each model. Addiscott (1993, 1994) and Burrough (1995) have thoughtfully suggested that the nature and intent of simulation models within the earth and ecosystem sciences ranges between two primary goals:

- 1) to develop decision support tools for resource managers
- 2) to increase our understanding of the interactions and mechanisms that affect processes within the landscape.

Addiscott (1994) terms decision support models as "functional" models, in contrast to process level "mechanistic" models. Typically, functional models require less explicit data inputs and rely on conceptualizations or abstractions to simplify the complex mix of physical and biological processes that exist in nature. Functional models often incorporate some mechanistic approaches, thus the distinction between the categories is often based on the intent rather than the exact algorithms within the models.

We will describe a number of mechanistic approaches to buffer zone modelling that can be used to examine and quantify site-specific processes at daily time scales. These approaches are linked by their requirements for intensive and often expensive data collection. To capture the functions and processes within a buffer zone, mechanistic models can be applied and compared to selected intensively monitored reference buffer zones to permit evaluation of the appropriateness of our process level understanding to real-life situations. Ideally, reference buffer zones would be located in a variety of climatic and hydrogeomorphic settings (Brinson, 1995). We suggest that mechanistic approaches are needed to establish the governing principles surrounding buffer zone processes. Our challenge is to find the lessons within the mechanistic models, honouring those insights while creating modelling approaches that recognize the limits imposed by the paucity of site-specific data.

How do we assess the accuracy of our models? Great controversy surrounds the issue of validation of landscape scale models (Addiscott, 1993). Bredehoeft and Konikow (1993) have suggested that we term our evaluation procedures "history matching", rather than validation. In this fashion we acknowledge that our model has agreed with measurements from a fixed set of situations and may not be suitable for all purposes. The evaluation of process-level models is confounded by the fact that many properties have high spatial and temporal variation. We will describe methods that incorporate variability of model inputs, and permit a "risk assessment" approach to the model outputs.

PHYSICAL SETTING

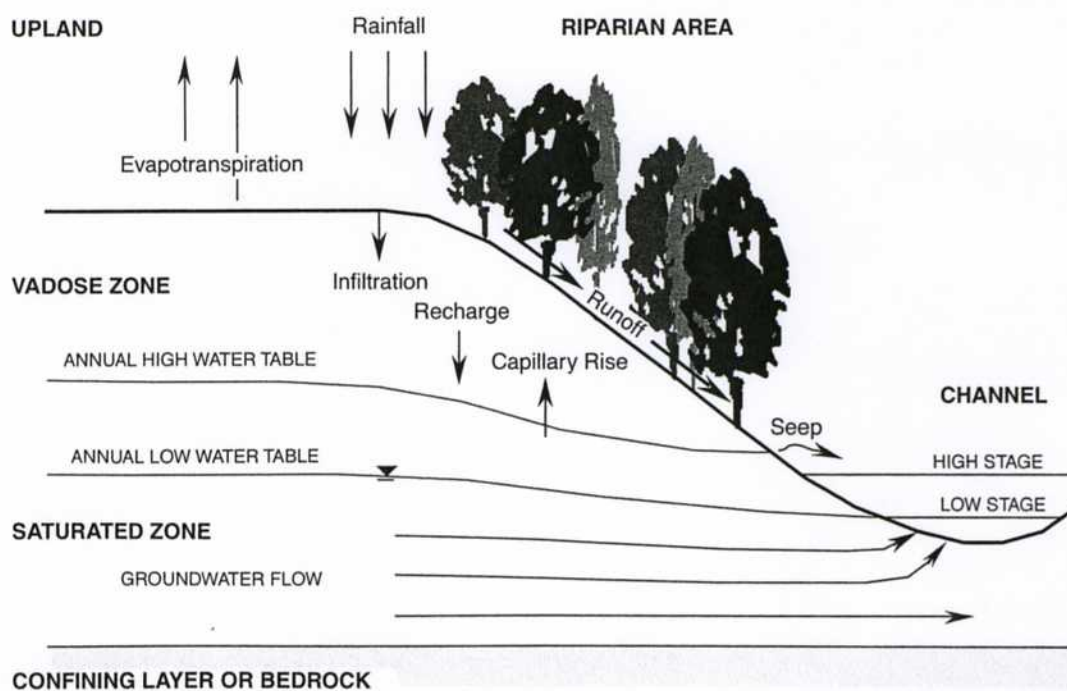
Our focus is on models that describe buffer zones located below upland areas and upgradient of open water bodies such as streams, rivers, lakes and estuaries. These areas are typically referred to as "riparian" zones, from the Latin word *ripa*, meaning bank or shoreline. In humid regions riparian areas typically receive groundwater and surface water from upland areas. The riparian buffer zone can influence the quantity, timing and quality of those waters prior to entry into concentrated flow channels or open water.

The riparian ecosystem extends laterally from an amorphous upland boundary to the open water. There are many ongoing investigations that are attempting to define the upland boundary of riparian zone functions as well as the soil depth at which transformation rates compare to those found in deep groundwater. Generally, investigators believe the unique properties of riparian zones are found within the upper 1-2 m of the soil (hereafter known as the biologically active zone) and extend upgradient to the limit of soils that show evidence of periods of partial saturation.

Many riparian zones occur on sites with shallow water tables; locations where the water table is within 0.1 – 1.5 m from the soil surface. The water table is the top of the groundwater, or in the language of the physicist (Hillel, 1980), the location at which the soil water is at atmospheric pressure. Above the water table the soil water is under tension from capillary suction, while below the water table the water is subject to hydrostatic pressures. The depth of the water table in relationship to the biologically active zone has extraordinary implications for the internal processes within a riparian buffer zone.

Waterborne materials enter a riparian ecosystem via surface runoff, groundwater flow and precipitation, and leave the ecosystem through evapotranspiration, percolation to deep groundwater, surface seeps and flow to surface waters (Fig. 1). Our models need to reflect the processes that influence the flow path and residence times in different portions of the riparian ecosystem. For example, infiltration alters the flow path from surface transport to groundwater transport. As a result, the fluxes of sediment and sediment-bound contaminants through the buffer zone are greatly reduced. Conversely, groundwater that emerges in surface seeps will rapidly traverse a buffer zone and bypass most attenuation processes.

Figure 1. Schematic diagram of the hydrological cycle of a riparian buffer zone.



MODELS OF SOIL MOISTURE IN THE UNSATURATED ZONE

Elevated soil moisture is the hallmark of riparian buffer zones. Soil moisture can be expressed in several formats. On a volumetric basis:

$$\theta_v = V_w/V_t \quad (1)$$

where:

θ_v = volumetric water content (cm^3/cm^3)

V_w = volume of water (cm^3)

V_t = total volume of the soil (cm^3)

and as % water-filled pore space:

$$\text{WFP} = \theta_v/\phi * 100 \quad (2)$$

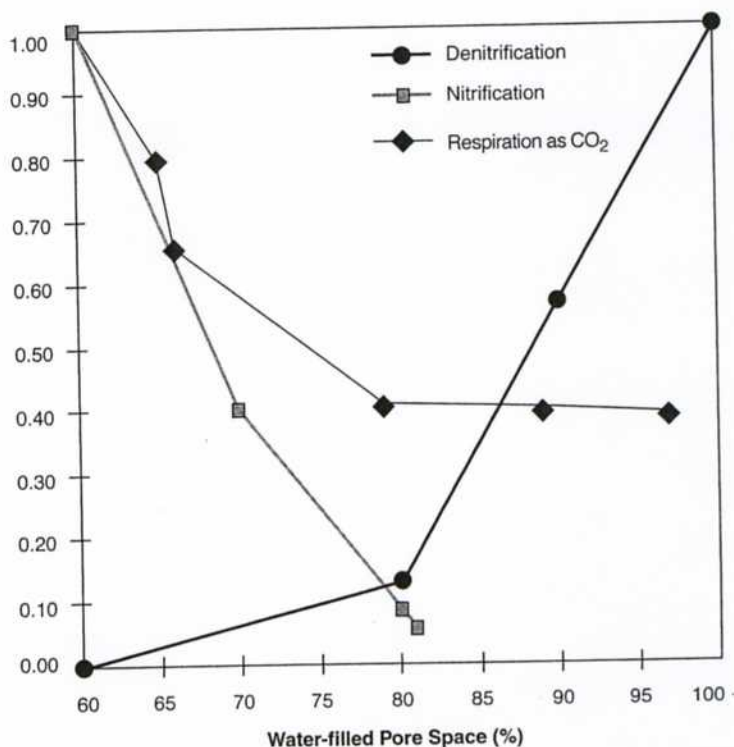
where:

WFP = % water-filled pore space

ϕ = total porosity (cm^3/cm^3).

Many internal processes within riparian ecosystems emanate from the temporal and spatial patterns of soil moisture within the biologically active zone of the soil. Linn and Doran (1984) related the relative potential for aerobic and anaerobic microbial activity to the WFP in a soil (Fig. 2). They concluded that the rate of many soil microbial activities, including nitrification, denitrification and respiration, is strongly influenced by WFP. In particular, relative microbial activity was extremely sensitive to WFP in the range between 60-100%. For example, in Figure 2, the relative denitrification rate within a soil increases 5-fold when the WFP increases from 80% to 90%.

Figure 2. Relationships of water-filled porosity versus selected microbial transformation rates. These relationships are commonly used in models of soil biogeochemistry. Adapted from Linn and Doran (1984).



Although Groffman and Tiedje (1988) have suggested that the relationships between WFP and microbial activity vary during wetting and drying cycles, several well-recognized soil biogeochemical models, such as the CENTURY model (Parton *et al.*, 1988) and the just-released REMM model (Altier *et al.*, in prep.) rely on the insights and relationships of Linn and Doran (1984) to modify microbial transformation rates based on WFP.

In addition to microbial processes, soil wetness can influence other processes, including the redox potential, infiltration rate, root uptake, evapotranspiration and the extent and timing of water table fluctuations. Thus, the ability to predict temporal and spatial patterns of WFP is central to explicit models of internal processes in riparian buffer zones.

There are a large number of one-dimensional soil-moisture models in use to evaluate the fate and transport of agrichemicals in upland areas. Efforts are underway to adapt these models for use in riparian areas. We will first review the capacity-based approach. This approach is the core of simulation models such as GLEAMS (Knisel *et al.*, 1992), SLIM (Addiscott and Whitmore, 1991), NLEAP (Shaffer *et al.*, 1991) and PRZM (Carsel *et al.*, 1984). In upland situations these functional models have been found to generate reasonable agreement with more mechanistic estimates of water and solute flux through the soil profile. However, in shallow water table soils, several of the assumptions inherent in capacity-based models are likely to generate misleading results. We will present a mechanistic model, LEACHN (Hutson and Wagenet, 1992), that can address these complex soil water dynamics. Finally, we will highlight where capacity-based models need to be modified to address riparian situations and present a hybrid model DRAINMOD (Skaggs, 1991), that may serve as a starting point for future work.

Capacity-based models

Capacity-based models divide the soil profile into a series of horizontal layers or compartments and generate a daily water balance for each layer. The mass balance equation for each soil layer is:

$$SM_{ij} = F_{ij} + D_{ij} - ET_{ij} - O_{ij} + SM_{i(j-1)} \quad (3)$$

where:

SM_{ij} = soil moisture within layer i , on day j (cm)

F_{ij} = infiltration to layer i , on day j (cm)

D_{ij} = percolation received from drainage of upper soil layers on day j (cm)

ET_{ij} = plant and soil evapotranspiration from layer i , on day j (cm)

O_{ij} = drainage outflow from layer i , on day j (cm).

The volumetric water content (θ_v) of layer i , on day j is then computed as:

$$\theta_v = SM_{ij} / (\text{Vertical depth of soil layer } i) \quad (4)$$

Capacity models ascribe three tiers of water retention capacities to each soil layer. The maximum water storage is the saturation water content, equivalent to 100% WFP. Wet soil is expected to drain to "field capacity", an equilibrium condition that occurs following drainage of gravitational water. In most capacity models, field capacity is fixed through time at a moisture content that equates to the soil water retention at -0.33 bars potential. Finally, each soil layer is assigned a capacity that corresponds to the water content unavailable for plant uptake, known as "permanent wilting point". Given the importance of partial saturation to microbial activity rates, both the rate of drainage from a soil layer as well as the equilibrium water content following gravitational drainage require careful examination.

In early versions of capacity models, gravitational water (i.e., soil water content above field capacity) was assumed to drain from a layer in a single day. In order to mimic drainage patterns more realistically, Addiscott and Whitmore (1991) created a functional rate parameter, α , that limits

drainage to a set proportion of gravitational water each day. Through the use of this type of functional rate parameter, capacity models may be capable of providing some important insights into the temporal patterns of partial saturation within the biologically active zones of riparian buffers.

Capacity models recognize that infiltration is affected by soil moisture. Most models of infiltration, whether functional or mechanistic, rely on estimates of soil wetness of the surface layers to modify the infiltration rate for a given site. Drier conditions enhance infiltration, while wetter conditions may sometimes preclude infiltration or even contribute to overland flows via surface seeps. Common approaches that may be useful for riparian buffer zones are the Green-Ampt method and the Curve Number method (Rawls *et al.*, 1993).

Limitations of capacity-based models for riparian areas

As mentioned earlier, several assumptions inherent in capacity-based models do not match the soil-water dynamics in soils with shallow water tables:

1) Field capacity is a dynamic property in riparian soils

In sites with shallow water tables the soil moisture at any depth within the root zone is intimately linked to the depth of the water table. During periods of minimal evapotranspiration and infiltration the distribution of soil moisture in the unsaturated zone reaches an equilibrium with the water table in response to its pore size distribution and its distance above the water table. At equilibrium, soil water at a given location is held by a capillary tension equal to its vertical distance above the water table i.e., the potential pull exerted by gravity. Neglecting hysteresis, for a given soil, each capillary tension relates to a distinct soil water content. This relationship is known as the Soil Moisture Retention Curve (Hendrickx, 1990).

Figs. 3a & b illustrate the effect of the water table on the equilibrium water content at a depth of 20 cm within the same soil. When the water table is 100 cm from the surface, the equilibrium water potential and WFP are -80 cm (-0.08 bars) and 59% respectively. If the water table rises to 40 cm from the surface, the equilibrium potential and corresponding WFP would be -20 cm and 88%, respectively. Thus the potential for anaerobiosis in the unsaturated zone is much greater when the water table is 40 cm from the surface than when it is 100 cm from the surface — even when all other factors are unchanged.

Figure 3a. Soil water distribution and water potential at equilibrium conditions for a water table at 100 cm.

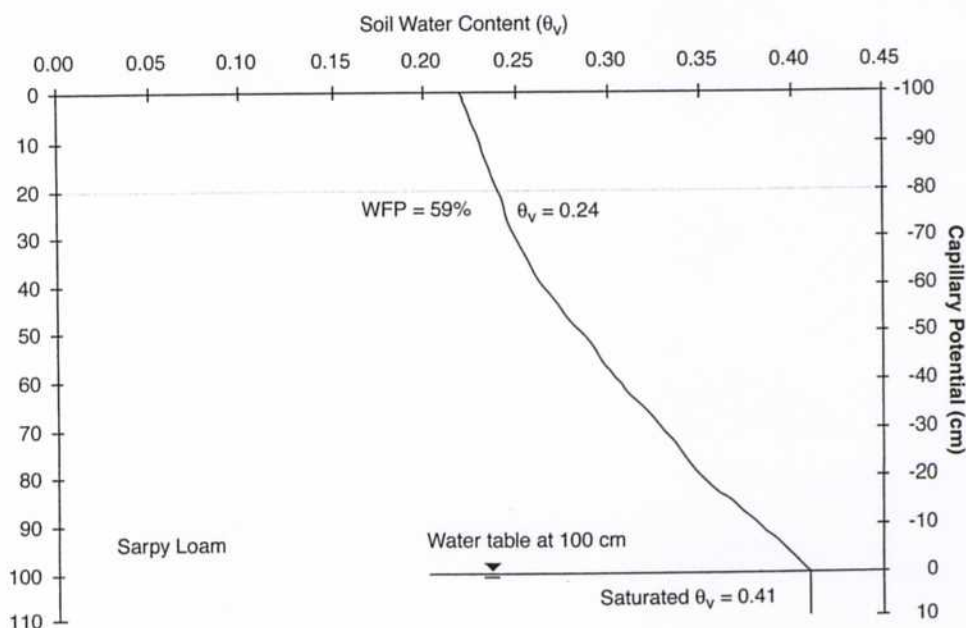
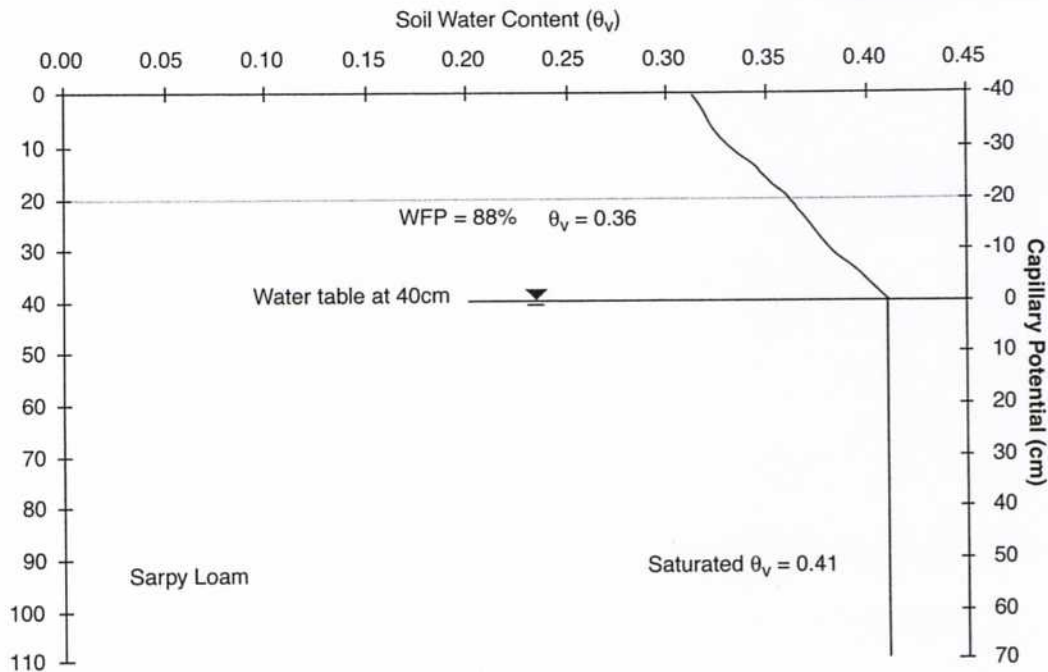


Figure 3b. Soil water distribution and water potential at equilibrium conditions for a water table at 40 cm.



2) *Upwelling of water from the water table can occur in response to evapotranspiration*

The presence of a shallow water table can affect the extent of water extraction and subsequent soil drying that results from evapotranspiration. Typical capacity-based soil moisture models incorporate a threshold soil moisture level to correspond to drought stress. Below this level, removal of soil moisture by evapotranspiration drops below non-stressed "potential" rates.

In upland situations, water extracted from the root zone is not expected to be replenished from greater depths and the soil moisture declines in direct response to evapotranspiration. However, in the presence of a shallow water table evapotranspiration can generate an upward flow of water to the root zone. The potential for upwelling results from a gradient between the drying soil within the root zone and the tension-free groundwater. The hydraulic conductivity of the media between the groundwater and the root zone is the dominant factor affecting the rate of upward flow. A version of the Darcy-Buckingham equation describes this upward flux:

$$q = K(\Psi) [(d(\Psi)/dz) - 1] \quad (5)$$

where:

q = flux (equal to evaporation rate under steady-state conditions)

$K(\Psi)$ = unsaturated hydraulic conductivity corresponding to a given soil moisture tension

Ψ = soil moisture tension

z = height above the water table.

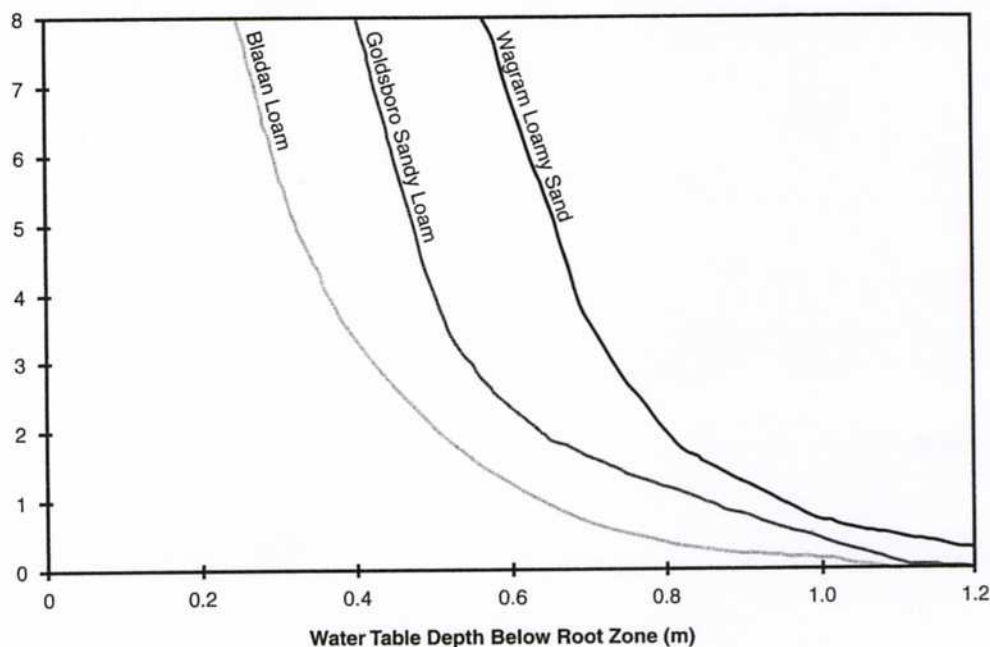
The Darcy-Buckingham equation modifies Darcy's equation to address flux within unsaturated media. It reflects the fact that hydraulic conductivity for a given soil horizon is greatest when the soil is saturated and declines as soil moisture declines.

Skaggs (1991) used a mechanistic approach similar to that outlined in equation (5) to generate the relationships between depth to water and upward flux for different soils in North Carolina (Fig. 4).

These types of analyses have demonstrated that a wide range of soils can generate considerable upward flux in response to an evaporating zone within 1 m of the water table (Hillel, 1980; Skaggs, 1991).

Figure 4. Effect of water table depth on steady upward flux from the water table for several North Carolina soils. From Skaggs (1991).

Darcy-Buckingham Predictions of Upward Flux for Three North Carolina Soils



Adapted from Skaggs (1991)

The occurrence of upwelling into the root zone demands that we incorporate several factors into our models of riparian zone dynamics. First, we must recognize that groundwater contaminants such as nitrate-N have the potential to move into the biologically active zone of the unsaturated zone. In that setting, nitrate-N will be subject to a host of biological transformations, including plant uptake, denitrification and immobilization. Second, because of upwelling, the entire soil horizon of riparian sites can remain considerably wetter than upland soils. In the presence of a shallow water table, the root zone will begin to dry only if the rate of evapotranspiration exceeds the rate of upwelling into the root zone. As a result, we need to adjust the common capacity-based approaches to soil moisture balance simulations to reflect the fact that minimal drying may result from evapotranspiration.

Mechanistic models of soil moisture

Mechanistic models, e.g. LEACHN (Hutson and Wagenet, 1992), have been developed to simulate the movement of water and solutes through soil profiles. Some of these models use daily or hourly climatic records and permit evaluations of flux in response to seasonal and annual fluctuations. These models rely on the Darcy-Buckingham equation in combination with the continuity equation to generate soil moisture flux in the unsaturated zone. Models can simulate the full suite of conditions that occur in soil with shallow water tables. The key data requirements are soil hydraulic properties, particularly the soil moisture retention curve (θ vs. Ψ) and the relationship between hydraulic conductivity and volumetric water content (K vs. Ψ).

Several excellent reviews (Hendrickx, 1990; Rawls *et al.*, 1993; Mualem, 1986) describe the use of field, laboratory and statistical techniques to estimate soil hydraulic properties. The soil moisture retention

curve is often generated in the laboratory with a variety of devices that induce a series of known pressures or suctions on undisturbed soil samples. The samples usually start at a saturated condition and are weighed after reaching equilibrium with each succeeding pressure or suction. Hanging water columns are used in combination with sand tables or pressure cells to simulate near saturated conditions. For greater tensions, some type of pressurized chamber is required. Occasionally, the soil moisture retention curve is obtained under field conditions. This approach can be extremely time-consuming and requires the use of non-destructive monitoring methods, such as time domain reflectometry in combination with tensiometers. Both laboratory and field methods are time and labour intensive.

The relationship between K and Ψ is even more difficult to obtain directly from field and laboratory measurements. As a result, hydraulic properties of soils are often generated from pedotransfer functions (Bouma and van Lanen, 1987; Bouma *et al.*, 1996). Pedotransfer functions relate soil hydraulic properties to more easily measured soil properties, such as texture or the saturated hydraulic conductivity. In general, all of these relationships are recommended for use with generic classes of soils, rather than for site-specific analyses. More reliable pedotransfer functions have also been developed which use selected field measurements of soil hydraulic properties to generate the full range of relationships between K and Ψ and between Ψ and θ (van Genuchten *et al.*, 1991).

An additional difficulty associated with the prediction of soil moisture in the unsaturated zone is that the soil moisture retention curve does not follow the same pattern during periods of drainage or wetting. This phenomenon, known as hysteresis, theoretically can have a large influence on the capillary fringe above the water table (Jaynes, 1990). Very limited information is available on the extent of hysteresis in soils and the incorporation of algorithms that describe hysteresis would add great complexity to soil water models.

WE NEED TO INCORPORATE VARIATION INTO OUR MODELS

We have argued that riparian buffer zone models need to be highly sensitive to the location of the water table and to soil hydraulic properties in the unsaturated zone. Yet, both of these characteristics can display a high degree of spatial variability, particularly since riparian areas are transition areas between uplands and open water. In addition to spatial variation, the water table depth and corresponding responses in the unsaturated zone will exhibit seasonal trends that are confounded by intermittent recharge events (Haycock and Pinay, 1993).

The soil moisture models we have described simulate processes at a point scale, based on assumptions of Darcian flow. These types of models have come under well-deserved criticism for their failure to describe the range and complexities of landscape-scale processes. Of additional note is the fact that we often aggregate selected areas of land into classes of similar characteristics and select a single value to represent the input parameters of the aggregated area (Beven, 1989). However, within a soil mapping unit the soil hydraulic properties are notoriously variable at the point scale (Warrick and Nielson, 1980). Soil survey maps are the most available source of input data for buffer zone modellers. Yet, Simmons *et al.* (1992) found large variation in the water table elevation within a single soil drainage class aggregate of a soil survey map, suggesting that the resolution of standard soil maps (13 m at a scale of 1:15,840) may be too coarse to incorporate important differences between soil classes.

Hence, any deterministic approach may create a misleading picture of the magnitude and relative importance of different riparian processes. Equally important, a deterministic approach ignores the need to quantify the level of uncertainty inherent in our simulations. We are likely to find that different types of buffer areas will vary in both the expected mean as well as in the variability of their water quality functions. Both of these factors will be of great use to decision makers who need to consider risk assessment in their management strategies (Bouma *et al.*, 1996).

Armed with the knowledge that critical inputs have a high degree of spatial and temporal variability, we should strive to build some level of stochastic evaluation into our modelling efforts. Monte Carlo

