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Appropriate vertical discretization of Richards' equation for two-dimensional watershed-scale modelling

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Abstract:

A number of watershed-scale hydrological models include Richards' equation (RE) solutions, but the literature is sparse on information as to the appropriate application of RE at the watershed scale. In most published applications of RE in distributed watershed-scale hydrological modelling, coarse vertical resolutions are used to decrease the computational burden. Compared to point- or field-scale studies, application at the watershed scale is complicated by diverse runoff production mechanisms, groundwater effects on runoff production, runon phenomena and heterogeneous watershed characteristics. An essential element of the numerical solution of RE is that the solution converges as the spatial resolution increases. Spatial convergence studies can be used to identify the proper resolution that accurately describes the solution with maximum computational efficiency, when using physically realistic parameter values. In this study, spatial convergence studies are conducted using the two-dimensional, distributed-parameter, gridded surface subsurface hydrological analysis (GSSHA) model, which solves RE to simulate vadose zone fluxes. Tests to determine if the required discretization is strongly a function of dominant runoff production mechanism are conducted using data from two very different watersheds, the Hortonian Goodwin Creek Experimental Watershed and the non-Hortonian Muddy Brook watershed. Total infiltration, stream flow and evapotranspiration for the entire simulation period are used to compute comparison statistics. The influences of upper and lower boundary conditions on the solution accuracy are also explored. Results indicate that to simulate hydrological fluxes accurately at both watersheds small vertical cell sizes, of the order of 1 cm, are required near the soil surface, but not throughout the soil column. The appropriate choice of approximations for calculating the near soil-surface unsaturated hydraulic conductivity can yield modest increases in the required cell size. Results for both watersheds are quite similar, even though the soils and runoff production mechanisms differ greatly between the two catchments. Copyright © 2003 John Wiley & Sons, Ltd.

KEY WORDS hydrology; hydrological modeling; Richards' equation; GSSHA; CASC2D; spatial convergence; vadose zone

INTRODUCTION

The Richards' equation (RE) (Richards, 1931) is the most general method to compute soil moistures and hydrological fluxes, such as infiltration, infiltration excess, evapotranspiration (ET) and groundwater recharge. Commonly encountered field conditions, such as soil layering, shallow groundwater table and the effect of soil moisture on infiltration, are easily incorporated into the RE model solution. There is no requirement that the runoff production mechanism be known a priori or limited to one type, as RE can be used to calculate runoff resulting from infiltration excess and saturation excess mechanisms, which can occur simultaneously in different areas of a watershed.

Simpler, approximate methods of calculating infiltration, such as the widely used Green and Ampt (1911) method, allow special cases of infiltration to be approximated. Modifications of simple infiltration models

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(Clapp, 1982; Chu, 1997; Ogden and Saghafian, 1997; Wang and Hjelmfelt, 1998) extend the applicability of these models, but they remain limited by their basic assumptions. As the complexity of these approximations increases, the computational advantage in their use diminishes (Short *et al*., 1995). The RE should be applied when the assumptions used in simpler methods are invalid or when soil moisture profiles and vertical fluxes of water in the unsaturated zone are needed (Downer and Ogden, 2003a).

Although offering potential benefits, applying RE in surface water hydrological models has drawbacks. The RE can be computationally expensive when used to describe sharp wetting fronts during infiltration (Ross, 1990; Pan and Wierenga, 1995), and RE has long been considered too computationally expensive for calculating water movement in variably saturated soils in the context of general surface water hydrology (Ross, 1990; Smith *et al*., 1993; Short *et al*., 1995, Corrandini *et al*., 1997). The availability of inexpensive, high-power computers has resulted in several models that use RE to compute soil moistures, infiltration, infiltration excess, ET and groundwater recharge (Abbott *et al*., 1986a,b; Dawes and Hatton, 1993; Refsgaard and Storm, 1995; van Dam and Feddes, 2000).

NUMERICAL ISSUES IN INCORPORATING RICHARDS' EQUATION IN HYDROLOGICAL MODELS

Unlike simpler methods of computing hydrological fluxes, general solution of the partial differential equation (PDE) described by Richards (1931) requires that finite difference, finite volume or finite element techniques be used. According to the Lax Theorem (Richtmyer and Morton, 1967) numerically stable solution schemes consistent with linear PDEs also converge. This rule is generally accepted for non-linear PDEs, such as RE, although it not yet proven (Tannehill *et al*., 1997). In a spatial convergence study, the cell size is varied to determine the effect of cell size on model response. If a spatial convergence study can demonstrate that the model does indeed converge as resolution increases, then it also confirms that the solution scheme is both consistent with the PDE and numerically stable. A spatial convergence study also allows the determination of the resolution required to accurately represent the system. This is extremely important for the selection of parameter values in any physically based model. If the PDE used accurately describes the physical system, the model results will converge on a solution as the time and space increments used in the discrete approximation are refined. Conversely, if physically appropriate parameter values are used with coarser resolutions, the error in the model prediction increases. Values of parameters fitted for arbitrary discretizations run the risk of having no physical meaning because the amount of error in the numerical approximation of an exact PDE is unknown. If the model applied with the actual physical properties does not accurately reproduce the system response then either the discretization is too coarse, the numerical scheme is inconsistent with the PDE or the PDE does not actually describe the physical system. Usually, actual parameter values are not known and are estimated by calibration, the process of adjusting parameter values until observed and predicted results are similar. In the case of a PDE such as RE, calibration alone, without a spatial convergence study, can lead to compensation for errors in the numerical formulation of the model by the use of unrealistic parameter estimates. However, if the parameter values are to have actual physical meaning, then the error in the numerical formulation must be understood and minimized.

The need for fine vertical resolution in the solution of RE to simulate sharp wetting fronts into initially dry soils has been discussed by several researchers (Ross, 1990; Paniconi *et al*., 1991; El-Kadi and Ling, 1993). Smirnova *et al*. (1997) showed that the number of vertical grid cells used in RE to compute soil moistures for atmospheric modelling affects the soil moisture calculations. Van Dam and Feddes (2000) showed that small grid sizes are required to estimate hydrological fluxes with RE applied at the field scale. At the watershed scale, the application of RE is complicated by the effects of runoff, runon, spatial heterogeneity, fluctuating water tables and unsteady boundary conditions. If fine discretization is required to properly simulate hydrological fluxes then the failure to use sufficiently fine resolution may result in the inability to simulate these fluxes at the watershed scale using realistic parameter estimates. Although the issue of assigning appropriate parameter values for different scales in hydrological modelling in general (Bergstrom and Graham, 1998; Moglen and

Hartman, 2001), and in physically based hydrologic models in particular (Ewen *et al.*, 1999; Molnar, 1997; Sanchez, 2002), has been the topic of much discussion by several researchers, the application of RE within the framework of distributed hydrological modelling presents an interesting case of a numerical method application within a distributed overland modelling framework. The question is how the spatial resolution and parameterization of RE affects the overall watershed model results.

In this study we investigate the applicability of RE for general watershed-scale hydrological modelling by applying the distributed, physically-based Gridded Surface Subsurface Hydrological Analysis (GSSHA) model (Downer and Ogden, 2003b) at two very different watersheds: the Hortonian runoff (Horton, 1933) dominated Goodwin Creek Experimental Watershed (GCEW) in northern Mississippi, and the non-Hortonian groundwater-dominated Muddy Brook watershed in northeastern Connecticut. We investigate the vertical discretization necessary to properly simulate surface hydrological fluxes and examine the effect of vertical discretization on parameter assignment and sensitivity to parameter estimates. By applying the model in both Hortonian and non-Hortonian basins we are able to identify the effect of dominant runoff production mechanisms on required RE discretization. We also investigate methods to increase the applicability of RE in general watershed modelling by increasing computational efficiency.

THE GSSHA MODEL

The GSSHA model is a reformulation and enhancement of CASC2D version 1·18b (Ogden, 2000; Ogden and Julien, 2002) for the Watershed Modelling System (WMS) (Nelson, 2001). The process based GSSHA model simulates two-dimensional overland flow, one-dimensional channel routing, two-dimensional saturated groundwater flow, canopy retention, microtopography, infiltration and ET using finite-difference and finite-volume methods. The purpose of the GSSHA model is to extend the capability of the CASC2D model to non-Hortonian watersheds, to allow for the simulation of groundwater/surface-water interaction, and to accurately model soil moistures in the unsaturated zone. The GSSHA model uses a one-dimensional finite-difference solution of RE to simulate the unsaturated zone. The unsaturated zone can be linked to a two-dimensional finite-difference representation of the saturated groundwater flow. Downer (2002) gives a complete description of the GSSHA model formulation.

Vadose zone modelling with RE

The vadose zone controls the flux of water between the land surface and groundwater and partitions rainfall into runoff, infiltration, groundwater recharge and ET. In GSSHA the unsaturated zone below each overland flow cell is simulated using the one-dimensional (vertical direction) head-based form of RE

$$C(\psi)\frac{\partial\psi}{\partial t} - \frac{\partial}{\partial z}\left[K(\psi)\left(\frac{\partial\psi}{\partial z} - 1\right)\right] - W = 0 \tag{1}$$

where C is the specific moisture capacity, ψ is the soil capillary head (cm), z is the vertical coordinate (cm) (downward positive), t is time (h), $K(\psi)$ (cm) is the effective hydraulic conductivity and W is a flux term added for sources and sinks (cm h^{-1}), such as ET and infiltration. The head-based form of RE is valid in both saturated and unsaturated conditions (Haverkamp *et al.*, 1977). Infiltration, evaporation and groundwater recharge can all be modelled without a change in variable with the head-based form of RE.

In GSSHA the soil column is subdivided into discrete cells and RE is solved using a cell-centred implicit finite-difference numerical algorithm. The solution scheme is central-difference in space and forward-difference in time and is thus second-order accurate in space, first-order accurate in time. After solving for heads in each cell, flux updating synchronizes the heads and soil moistures, and improves the mass balance (Kirkland, 1991; Kirkland *et al.*, 1992). During and following rainfall events the maximum time-step allowed in the RE solution is the overall model time-step, generally about 1 min. Once overland flow routing is completed the ET model step, 1 h, becomes the maximum RE model time-step. Model stability and accuracy is increased by internally limiting the RE time-step based on a maximum change in water content, as suggested by Belmans *et al*. (1983). Values of K across the faces of cells, intercell K, are computed from the cell-centred values on each side of the interface. Intercell K may be calculated using either an arithmetic or geometric average.

RE solution boundary conditions. The upper boundary condition varies depending on surface ponding. Ponding occurs when there is more water on the soil surface than can infiltrate during a computational time-step. The upper boundary condition on the solution domain is either a specified flux if there is no surface ponding, or a specified pressure (head) when ponding occurs. The determination of the proper upper boundary condition is determined each time-step internally in the program.

Three different lower boundary conditions can be specified. First, when the groundwater table is far from the soil surface, such as in the case of well-drained soils, a zero head-gradient lower boundary condition is appropriate. Second, the lower boundary can be a static water table, where the elevation of the top of the last cell in the soil column is equal to the elevation of the saturated water table. The pressure at the top of the cell is zero, and the cell-centered pressure is equal to half the cell size. Third, when two-dimensional saturated groundwater flow is simulated in GSSHA, the lower RE boundary condition is a dynamic groundwater table. In this case, the size of the last non-boundary cell and the number of cells changes as the water table rises and falls.

Non-linear coefficients. Variables K and C from Equation (1) are non-linearly dependent on the water content of each cell. Unless field data are available, the Brooks and Corey (1964) equations as extended by Huston and Cass (1987) are used to calculate K and C based on the water content of the cell. The dependence of K and C on water content makes RE highly non-linear. In GSSHA, RE is linearized by fixing values of C and K during each time-step. Another way to linearize the RE is to iterate on K and C during each time-step. Although iterating on the non-linear coefficients will almost always improve the solution and mass balance to some extent, iterations are not normally needed in GSSHA because the flux-updating technique is used (Kirkland, 1991; Kirkland and Hills, 1992). One exception occurs when there are saturated cells in the soil column. As the flux-updating technique cannot be used in these or adjacent cells, mass balance problems are possible (Kirkland, 1991; Kirkland and Hills, 1992). Under ponded conditions saturated cells often appear and iterations are always performed when ponded conditions occur, resulting in improved accuracy and reduced mass-balance errors.

Hydrological flux computations. Potential ET (PET) is computed using the Penman–Monteith equation (Monteith, 1965). The PET is distributed over the root depth, which must be specified for each soil column. To determine actual ET (AET) for each cell within the root depth, PET is adjusted for the water content in each cell as described by Downer (2002). The AET is then applied to each cell in the root depth using the source term, W, in Equation (1). Groundwater recharge is computed as the flux across the last non-boundary cell in the soil column. Infiltration is computed as the flux across the surface of the first cell in the computational domain. Water remaining on the surface after computation of ET and infiltration may become runoff.

TEST CATCHMENTS AND MODEL REPRESENTATIONS

We use data and observations from two very different catchments to determine the impact of gross, site-specific watershed characteristics on the appropriate watershed-scale application of RE within a distributed hydrological modelling framework. These two catchments were selected because they have different primary runoff production mechanisms, and research-quality data sets have been collected at each site. This section briefly describes each catchment to illustrate their differences.

The Goodwin Creek Experimental Watershed (GCEW) is a 21·2 km^2 agricultural watershed located in northeast Mississippi, near the town of Batesville. A detailed description of the study watershed is provided in Alonso (1996). There are four main land uses in the catchment: active cultivation (14%), pasture (44%), forest (27%) and gullied land (15%) (Blackmarr, 1995). Soil textures in the watershed consist of silt loam (80%), clay loam (19%) and sand (1%). The elevation of the watershed ranges from 68 m to 127 m. The channels in the watershed are incised 2 to 3 m, and measurements of groundwater levels taken adjacent to the main channel show that the groundwater table is several metres below the ground surface. Base flow at the catchment outlet is typically less than 0·05 $m^3 s^{-1}$ (0·0023 $m^3 s^{-1} km^{-2}$) year round. Senarath *et al.* (2000) stated that these watershed characteristics, taken together with the predominance of fine soil textures, indicate that the infiltration-excess runoff production mechanism is dominant at GCEW. Soil moisture sensors installed in 1999 at two locations verify that runoff is produced by the Hortonian mechanism, particularly during the growing season (Downer and Ogden, 2003a).

The GCEW has been monitored continuously since 1981 by the United States Department of Agriculture Agricultural Research Service (USDA-ARS) National Sedimentation Laboratory (NSL). Data collected by NSL include precipitation, discharge, hydrometeorological variables and soil moisture. A network of 31 rain gauges records precipitation at GCEW. Channel discharge measurements are taken at 14 engineered structures located at subcatchment outlets. Soil moisture data are collected at two Soil Climate Analysis Network (SCAN) sites. Figure 1 shows the location of precipitation and discharge measuring stations, the SCAN sites, and the channel network at GCEW.

The second test catchment is the 3·64 km^2 Muddy Brook watershed, located near the northeastern Connecticut town of Ellington. The watershed is covered by forest (54%), suburban development (23%), pasture/hay fields (12%) and corn fields (11%) (Heng, 1996). Elevations in the watershed range from 123 to 60 m. Soils in the watershed are described as silty and sandy loams (Ilgen *et al.*, 1961). A 40 to 65 cm layer of stratified drift with saturated hydraulic conductivity (K_s) between 5 and 38 cm h^{-1} is located atop glacial till of lower hydraulic conductivity, 0·125–31 cm h^{-1} (Clausen *et al.*, 1993; Mullaney, 1995; Semagin, 1996). Bedrock, consisting of weathered Jurassic limestone, is located 2·7 to 6·7 m below the land surface (Clausen *et al.*, 1993). Near the stream the groundwater table is typically shallow, within 0·5 to 1·2 m of the land surface (Clausen *et al.*, 1993). Groundwater discharge to the stream was estimated by Mullaney (1995) to be approximately 0·000 002 $m^3 s^{-1}$ per metre of stream length. Data from Semagin (1996) indicated that base flow at the catchment outlet is typically less than 0·015 $m^3 s^{-1}$ (0·0041 $m^3 s^{-1} km^{-2}$). Note that the base flow per unit area is two times larger at Muddy Brook than at the GCEW.

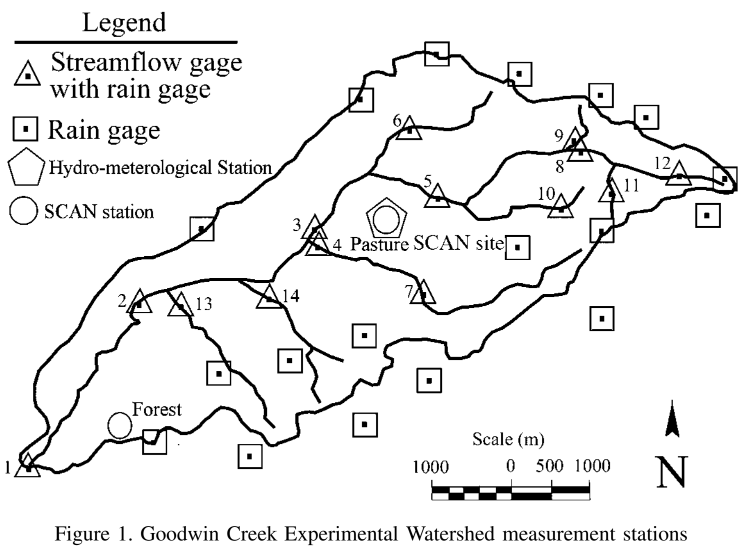

Figure 1. Goodwin Creek Experimental Watershed measurement stations

Research quality hourly rainfall, outlet discharge and groundwater level data are available for the period 29 June 1994 to 31 December 1994 (Semagin, 1996). The locations of measurement sites within the Muddy Brook watershed are depicted in Figure 2. Hydrometeorological data were collected at the nearby town of Stafford. A description of the hydrometeorological station is presented in Geigert *et al*. (1994). More complete descriptions of the Muddy Brook hydrology are available in Heng (1996), Semagin (1996) and Downer (2002).

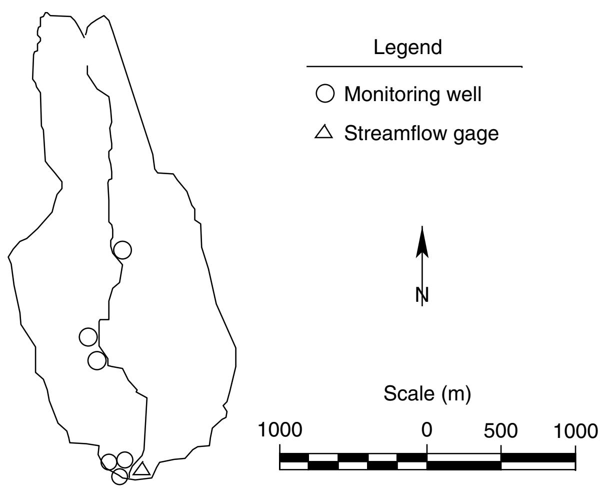

Figure 2. Muddy Brook measurement stations

Table I. Model descriptions for GCEW and Muddy Brook watersheds

Variable	Model attribute	GGEW	Muddy Brook
General	Grid size (m)	125	90
	X–Y grid cells (number)	1357	449
	Overall model time-step (s)	60	60
Precipitation	Rainfall distribution	Theissen polygon	Uniform
	Gauges (number)	31	1
Evapotranspiration	Method	Penman Monteith	Penman Monteith
	Root depth (m)	Equal to vegetation height	Equal to vegetation height
	Parameter assignment	Distributed by STLU	Distributed by STLU
Soil moistures and fluxes	Method	RE	RE
	Soil column depth (m)	1·0	Depends on water table
	Non-linear coefficients	Brooks and Corey	Brooks and Corey
	Intercell K	Geometric	Geometric
	Lower Boundary	Well drained	Water table surface
	Maximum $\Delta\theta$ during Δt	0·025	0·025
	Parameter assignment	Distributed by STLU	Distributed by STLU
Overland flow	Method	Two-dimensional diffusive wave	Two-dimensional diffusive wave
	Solution	ADE	ADE
	Surface retention	Distributed by land use	NA
	Roughness	Distributed by land use	Distributed by land use
Channel flow	Method	One-dimensional diffusive wave	One-dimensional diffusive wave
	Cross Sections	Trapezoidal	Trapezoidal
	Roughness	Uniform	Uniform

Table I. (*Continued*)

Variable	Model attribute	GGEW	Muddy Brook
Saturated groundwater	Method	NA	Two-dimensional Lateral flow
	Solution	NA	LSOR
	Groundwater time-step (s)	NA	720
	LSOR value	NA	1·0
	Watershed boundary type	NA	Head
	Interaction with stream	NA	Darcy Flux, uniform K_{rb} and M_{rb}

LSOR, line successive over relaxation; RE, Richards' equation; STLU, soil type/land use; ADE, alternating direction explicit; K_{rb}, hydraulic conductivity of river bed material; M_{rb}, thickness of river bed material.

Given that the importance of saturated groundwater is different in the two study watersheds, GSSHA is run with different options on each watershed. Groundwater discharge to the stream comprises a major portion of the stream flow at the Muddy Brook watershed (Semagin, 1996). Therefore, representation of the shallow water table is an essential part of the GSSHA model applied at Muddy Brook, and the lower boundary condition for RE is the saturated water table. Because GCEW has been determined to be Hortonian, at least during the time period of this study, there is no need to simulate saturated groundwater in this watershed and the lower boundary condition for RE is a well-drained soil (no change in soil pressure head boundary). Table I summarizes the model options used in simulating the two basins.

Initial parameters in both watersheds were assigned based on the soil type, land use, and combination soil type/land use (STLU) classifications. Overland hydraulic properties were assigned based upon land use. Soil hydraulic properties and ET parameters were assigned based upon the STLU. At GCEW initial parameter values were taken from Senarath *et al.* (2000), who used the CASC2D model with the Green and Ampt with Redistribution (GAR) method (Ogden and Saghafian, 1997) to calculate infiltration. Ogden and Saghafian (1997) showed GAR to compare favourably with RE for calculating infiltration in the case of multiple pulses of rainfall on fine textured, well-drained soils. Initial parameter values for Muddy Brook were assigned based on standard literature values (Rawls *et al.*, 1982) and from site-specific information (Ilgen *et al.*, 1961; Clausen *et al.*, 1993; Semagin, 1996).

NUMERICAL STUDIES

Vertical resolution RE convergence studies are conducted to demonstrate that the methods used are consistent and numerically stable. The vertical resolution convergence studies also reveal the required discretization to accurately simulate watershed-scale hydrological fluxes. Both uniform and spatially varied discretizations are explored. The sensitivity of model output to the estimates of model parameters, as related to vertical cell size for solution of RE, is also investigated. The RE is applied at the GCEW using a zero head-gradient lower boundary condition, and the Muddy Brook watershed is simulated with two different lower boundary conditions: static groundwater table and fluctuating water table. These different representations of the unsaturated zone allow determination of the influence of the lower boundary condition on solution accuracy.

The cells near the soil surface are thought to control rainfall partitioning. If so, coarser discretizations may be used at greater depths in the soil column. If conditions near the surface control the computation of hydrological fluxes, then alternative methods of calculating the non-linear coefficients used in RE at the soil surface may provide a means to increase cell sizes near the surface without significantly affecting model results or parameter estimates.

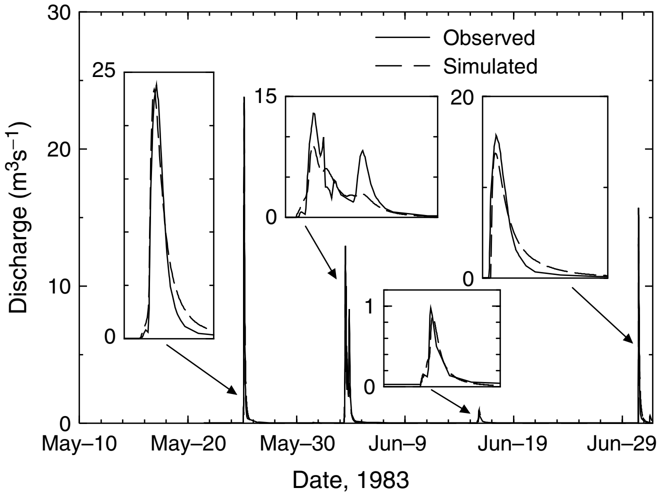

Figure 3. Observed and simulated Goodwin Creek Experimental Watershed outlet hydrograph during the test period

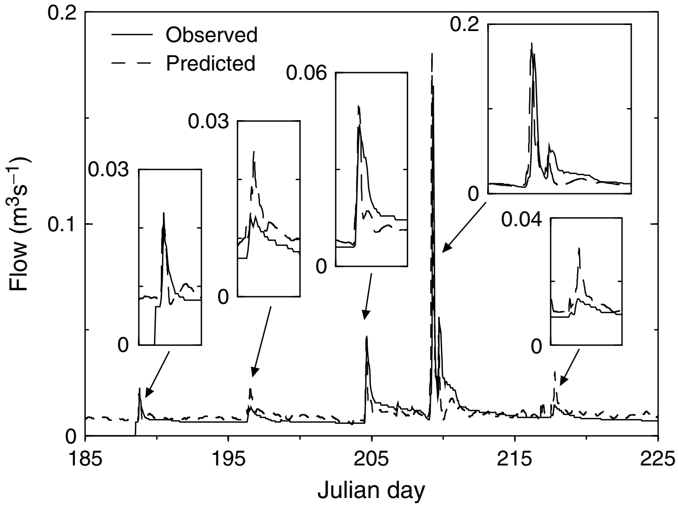

Figure 4. Observed and simulated Muddy Brook outlet discharge hydrograph during the test period

At GCEW a 6-week period of record is simulated, from 22 May through to 30 June 1982 (Figure 3). During this period, there are ten storm events, four of which produce peak discharges greater than 0·05 m^3 s^{-1}, which Senarath *et al.* (2000) determined is the smallest event value that allows accurate determination of event volumes at this site. The Muddy Brook watershed is simulated for the period 14 June through 14 August 1994 (Figure 4). This period contains 12 rainfall events. All numerical studies are conducted using parameter values determined through a preliminary calibration using arbitrary cell sizes. An automated process is used to determine final parameter values after determining the most efficient cell size distribution in each watershed. The calibration process and parameter values used to produce the simulated results in Figures 3 and 4 are discussed after a presentation of the various numerical tests conducted.

Uniform discretization spatial convergence

At GCEW the vertical discretization for each soil column is varied from 0·1 to 100·0 cm. This reduces the number of computational points in the unsaturated zone from 1 357 000 to 1357. The uniform vertical RE discretization in the top 1·0 m of soil at Muddy Brook is varied from 0·2 to 50·0 cm. At Muddy Brook, additional cells, ranging in size from 10·0 to 50·0 cm, are required below the top 1·0 m of soil and above the specified water table. The number of computational points in the unsaturated zone varies from 290 349 to 65 114. Spatial convergence is evaluated in terms of changes in volumes of: total infiltration, total discharge and total evaporation over the entire simulated period.

Results of the convergence study for infiltration, runoff and ET are shown in Figure 5. At Muddy Brook the observed outflow contains both surface water and groundwater components; only surface runoff from saturated source area and infiltration-excess runoff is shown in Figure 5. Model results with the smallest cell size, at the left-hand side of the figure, are assumed to be the correct solution. As seen in Figure 5, the GSSHA model predictions converge on a solution for infiltration, runoff and ET as the cell size decreases. The amount of infiltration is seen to be highly dependent on the vertical discretization used in the model. As the vertical cell size increases the amount of infiltration decreases, resulting in greater runoff. Total ET is less sensitive to the vertical resolution in the RE model. Evapotranspiration is highest for small cell sizes, decreases until the cell size exceeds 5 cm, and then increases with increasing cell size.

The relative change in infiltration, runoff and ET volumes with respect to rainfall for each increase in cell size is shown in Table II. As shown in the table, increasing the grid size to 0·5 cm results in only small changes in the model predictions, whereas the use of larger cell sizes has a much greater effect in both watersheds. Although only the results for geometric weighting are presented here, changing the averaging method to arithmetic with backwinding, as suggested by Lappala (1981) for infiltration modelling, did not change the dependence of hydrological fluxes on cell size.

Mass conservation is weakly related to cell size, increasing slightly with decreasing cell size. Table III presents the overall model mass conservation and the maximum event RE mass conservation error computed for each event from the time rainfall begins to the time overland flow ends. As can be seen in the table, mass is largely conserved for all cell sizes at both watersheds. Larger overall model mass balance errors at Muddy Brook are thought to occur because the lower boundary condition is the water table, which may result in saturated cells near the water table. This condition is known to cause problems with the flux updating procedure used in the model (Kirkland, 1991). This condition is exacerbated during periods between events because the time-step is large, 1 h, and no iterations occur unless water is ponded on the surface. These

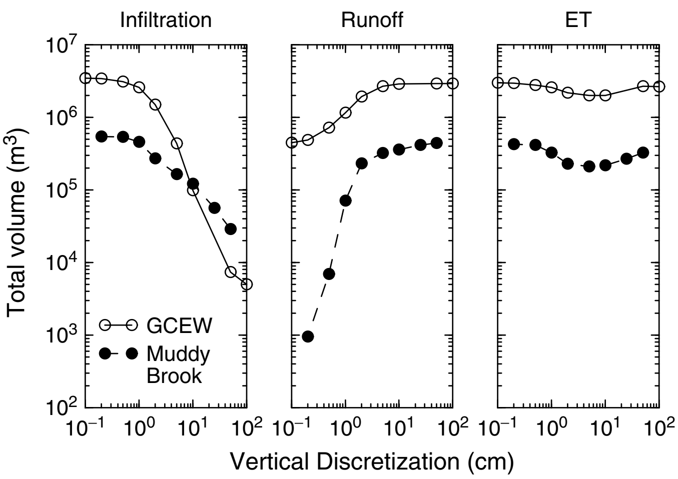

Figure 5. Uniform spatial convergence study results

Table II. Incremental change in hydrological fluxes expressed as a percentage of total rainfall

Cell size (cm)	GCEW Δ Infiltration	GCEW Δ Runoff	GCEW Δ ET	Muddy Brook Δ Infiltration	Muddy Brook Δ Runoff	Muddy Brook Δ ET
0·1						
0·2	−1·1	1·0	−0·9	—	—	—
0·5	−7·3	5·8	−4·4	−1·0	4·9	−1·7
1·0	−13·4	11·0	−5·2	−14·2	10·0	−16·4
2·0	−28·0	19·6	−10·4	−34·5	6·7	−17·6
5·0	−26·9	19·1	−4·5	−19·5	16·9	−3·7
10·0	−8·6	5·4	0·2	−8·0	29·5	1·5
25·0	−2·1	0·8	6·3	−12·1	11·8	9·4
50·0	−0·2	0·0	11·0	−5·1	1·1	10·7
100·0	−0·1	0·1	−0·9	—	—	—

Table III. Mass balance errors for uniform convergence studies

Δz (cm)	Overall mass error (%)		Maximum event RE error (%)	
	GCEW	Muddy Brook	GCEW	Muddy Brook
100·0	$<10^{-6}$	—	$<10^{-4}$	—
50·0	$<10^{-6}$	$1{\cdot}8 \times 10^{-1}$	$<10^{-4}$	10^{-4}
25·0	$<10^{-6}$	$1{\cdot}9 \times 10^{-1}$	$<10^{-4}$	$<10^{-4}$
10·0	10^{-6}	$1{\cdot}6 \times 10^{-1}$	$<10^{-4}$	$<10^{-4}$
5·0	$4{\cdot}3 \times 10^{-6}$	$1{\cdot}8 \times 10^{-1}$	$<10^{-4}$	$<10^{-4}$
2·0	$1{\cdot}6 \times 10^{-5}$	$1{\cdot}9 \times 10^{-1}$	$<10^{-4}$	$<10^{-4}$
1·0	$3{\cdot}2 \times 10^{-4}$	$1{\cdot}9 \times 10^{-1}$	$3{\cdot}0 \times 10^{-4}$	$<10^{-4}$
0·5	$4{\cdot}2 \times 10^{-3}$	$1{\cdot}4 \times 10^{-1}$	$2{\cdot}5 \times 10^{-3}$	$7{\cdot}9 \times 10^{-3}$
0·2	$2{\cdot}0 \times 10^{-2}$	$1{\cdot}9 \times 10^{-1}$	$3{\cdot}1 \times 10^{-3}$	3×10^{-4}
0·1	$3{\cdot}3 \times 10^{-2}$	—	$1{\cdot}1 \times 10^{-2}$	—

mass balance errors can be eliminated, or at least reduced, at the expense of increased computation time by specifying iterations on the non-linear coefficients regardless of surface conditions and/or specifying a smaller allowable maximum water content change per time-step. However, the errors are deemed acceptable. Event mass balance errors are typically of the order of 10^{-4} per cent at both watersheds.

Surface layer thickness

In the tests described above, each soil column is assumed to be uniform, with a uniform cell size used for the entire soil column. The GSSHA model allows the definition of three vertical soil layers in each soil column, representing the A, B and C soil horizons. The user must specify the thickness (cm) of each of the three layers, and also define the cell size that is used to discretize each layer.

In this test, the thickness of each of the three soil layers is varied during multiple simulations. In each simulation the cell size in the top layer is 0·2 cm. The cell size in the second layer is 0·5 cm and cell size in the third, bottom, layer is 1·0 cm. Several simulations are performed with different top-layer thickness of 1·0, 2·0, 5·0, 10·0 and 100·0 cm. The thickness of the second and third layers depends on the thickness of the top layer, as described in Table IV. The hydraulic properties of the soil, i.e. K_s, porosity (e), etc., are the same in each layer.

The GCEW is simulated over the same 6-week period, using the different surface soil-layer thicknesses. The results of these simulations are shown in Figure 6. Figure 6 shows the normalized total volume of infiltration, runoff and ET versus the thickness of the top layer with the fine resolution (0·2 cm). The flux

Table IV. Soil layers in GCEW surface soil layer thickness tests

First layer[a] thickness (cm)	Second layer[b] thickness (cm)	Third layer[c] thickness (cm)
1·0	39·0	60·0
2·0	38·0	60·0
5·0	35·0	60·0
10·0	30·0	60·0
100·0	0·0	0·0

[a] Cell size is 0·2 cm; [b] cell size is 0·5 cm; [c] cell size is 1·0 cm.

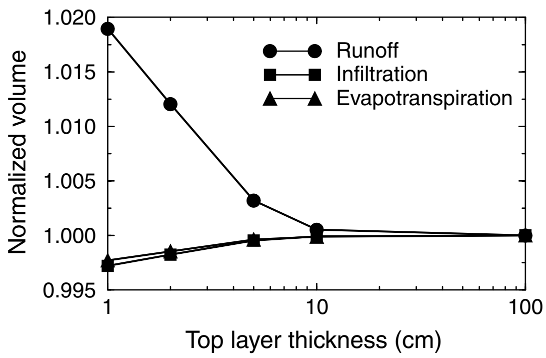

Figure 6. Influence of surface layer thickness on hydrological fluxes at GCEW

Table V. Effect of surface layer thickness on hydrologic fluxes expressed as percentage change from base condition

Top layer thickness(cm)	GCEW Δ Infiltration	GCEW Δ Runoff	GCEW Δ ET
100			
10	−0·01	0·05	−0·01
5	−0·05	0·32	−0·05
2	−0·18	1·21	−0·15
1	−0·28	1·89	−0·23

volumes are normalized by dividing the total volumes of infiltration, runoff and ET by the corresponding total volumes obtained from simulations where the entire soil column is finely discretized. The convergence study indicates that uniformly fine resolutions produce the correct solution. This semi-log plot indicates that values of infiltration, runoff and ET are not sensitive to the thickness of the surface layer, provided that this layer is finely discretized. As shown in Table V, differences in results between a 10·0 cm and 100·0 cm surface layer thickness are negligible. As shown in Figure 6, the difference is greater when the surface layer thickness is less than 10 cm, but results are still within 2% of the base model simulation results even when the surface layer is only 1·0 cm thick.

Importance of upper boundary condition

Predictions of hydrological fluxes using the ‘cell-centred’ soil moisture of the first cell in the soil column to calculate K at the soil surface, $K_{1/2}$, are compared with predictions of these same fluxes made using two alternative methods of computing $K_{1/2}$. The first alternative method assumes $K_{1/2} = K_s$ and is called the G&A method because Green and Ampt (1911) make this assumption in their famous infiltration formula. The second alternative assumes that $K_{1/2}$ is the geometric average of K_1 and K_s, and is called the 'average method'. The cell-centred method is always used to compute $K_{1/2}$ for a flux boundary condition. The two alternative methods are used only when the surface is ponded and the upper boundary condition is a head. The assumption in using these methods is that a very thin layer of soil is saturated at the soil surface, and that the water content at the centre of cell one is not the appropriate value to use to calculate $K_{1/2}$ under these conditions. The spatial convergence study is repeated using the two alternative methods.

The predictions of total infiltration, runoff and ET from these simulations are compared with the original predictions from GCEW in Figure 7 and from Muddy Brook in Figure 8. In this figure, model predictions obtained with the finest discretizations are assumed to be the correct solutions. As shown in Figures 7 and 8, in terms of calculating infiltration, the average method behaves similarly, but is less sensitive to the vertical discretization than the cell-centred method. The G&A method is quite insensitive to the vertical resolution. In terms of predicted runoff, Figures 7 and 8, the average method behaves similarly to the cell-centred method, but is less sensitive to the cell size. The G&A method produces approximately the same runoff as the average method until the vertical resolution reaches 1·0 cm. For cell sizes above 1·0 cm runoff continues to increase, but the results begin to diverge between the average and G&A methods. For larger cell sizes,

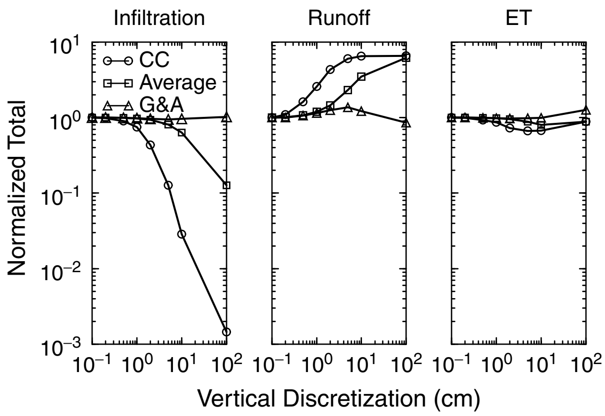

Figure 7. Influence of upper boundary condition on hydrological fluxes at GCEW

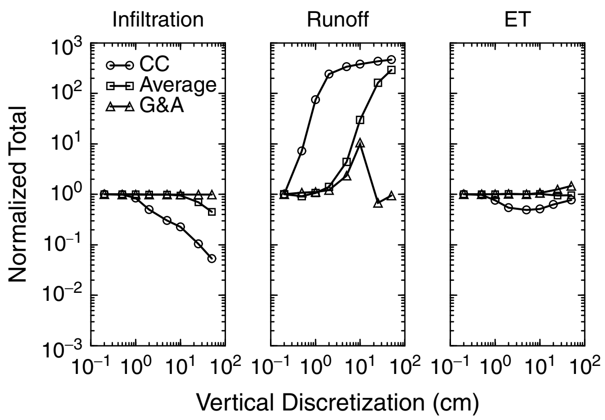

Figure 8. Influence of upper boundary condition on hydrological fluxes at Muddy Brook

above 5·0 cm at GCEW and 10·0 cm at Muddy Brook, the runoff actually decreases when the G&A method is used. The increased infiltration from the two alternatives results in greater actual ET owing to increased water contents near the soil surface. The average method generally results in more ET than the cell-centred method for intermediate cell sizes. The G&A method produces the same results as the average method until the cell size reaches 1·0 cm at GCEW, then the G&A and average methods diverge. At Muddy Brook the two methods result in essentially the same amount of ET until the cell size reaches 10·0 cm. As a result of greater infiltration, the use of the G&A method generally results in more ET than the other two methods.

In terms of deviation from the base discretization, for total hydrological fluxes, the alternative methods to compute $K_{1/2}$ allow the use of larger cell sizes compared with using the cell-centred method. The percentage change from the finest resolution for predictions with increased cell size is shown in Table VI for each alternative. If a 10% deviation from the base solution is considered the maximum allowable, maximum grid sizes at GCEW for infiltration, runoff and ET for the cell-centred case would be: 0·5, 0·2 and 0·5 cm, respectively. For the average method, the cell sizes could be increased to: 2·0, 0·5 and 5·0 cm, and for the G&A method: >100·0, 0·5 and 10·0 cm, respectively. For an application to predict runoff, the cell size could at least be increased from 0·2 to 0·5 cm resulting in a decrease in the number of computational nodes in the unsaturated zone from 678 500 to 271 400 at GCEW.

At Muddy Brook infiltration can be predicted within 10% of the finest resolution for cell sizes of 0·5 cm, 10·0 cm and >50·0 cm, for the cellcentered, average and G&A methods, respectively. Because the surface runoff is such a small percentage of the rainfall volume, small changes in infiltration cause large percentage changes in runoff. Still, cell sizes of 1·0 and 0·5 cm can be used with the average and G&A methods, respectively, and runoff predictions will still be within 10% of those obtained when using the finest discretization. For ET, the cell sizes can be greatly increased, the difference in ET from the base case using the average method was less than 5% for all cell sizes up to 50·0 cm. For G&A, ET could be predicted within 10% of the finest resolution with cell sizes up to 10·0 cm.

Sensitivity to parameter estimates

It is important to determine the effects of using discretizations larger than those suggested by the convergence studies on the assignment of parameter values. At GCEW the sensitivity of model predictions to parameter estimates is determined for two different vertical discretizations, the adequate discretization indicated by the convergence study for the cell-centred method, 0·2 cm, and a much larger resolution, which the convergence study indicates is inadequate for the cell-centred method, 2·0 cm.

Table VI. Percentage change in infiltration (Inf), runoff and ET and GCEW from base cases for alternative methods of computing K_r at the soil surface during surface ponding, i.e. cell-centered (CC), saturated (G&A) and average (Ave)

Watershed	Cell size	Inf CC	Inf Avg	Inf G&A	Runoff CC	Runoff Avg	Runoff G&A	ET CC	ET Avg	ET G&A
GCEW	0·2	−1·2	−0·1	−0·1	9·2	0·8	0·6	−1·2	−0·0	−0·1
	0·5	−9·6	−1·0	−0·9	61·3	7·3	6·2	−7·0	−0·7	−0·6
	1·0	−24·8	−2·6	−2·0	158·9	19·3	14·3	−13·8	−1·2	−1·3
	2·0	−56·7	−6·1	−3·5	332·4	44·7	25·4	−27·4	−2·7	−2·3
	5·0	−87·3	−18·7	−5·3	501·1	132·6	37·2	−33·3	−8·2	−2·0
	10·0	−97·1	−36·3	−3·6	548·7	248·2	21·6	−33·0	−10·2	−0·3
	100·0	−99·8	−87·3	2·11	557·8	517·5	−14·6	−11·4	−11·9	26·8
Muddy Brook	0·5	−1·0	0·1	−0·1	627·0	−7·5	8·5	−2·2	0·8	0·0
	1·0	−15·3	0·0	−0·1	7365·0	6·3	11·3	−23·2	1·3	0·6
	2·0	−49·9	0·0	−0·1	24251·1	42·0	21·8	−45·8	2·5	2·0
	5·0	−69·4	−0·6	−0·3	33915·0	342·6	133·6	−50·5	0·7	0·4
	10·0	−77·5	−5·2	−1·3	37725·6	2893·3	893·0	−48·6	2·4	6·4
	25·0	−89·6	−30·2	0·1	43481·8	16112·7	−32·1	−36·6	−4·6	25·7

Sensitivity of model output to changes in model parameters is determined by varying input parameters by ±25%. The sensitivity of the model is analysed with respect to the following RE parameters: K_s, bubbling pressure (ψ_b), pore distribution index (λ), wilting-point water content (θ_{wp}), e, initial water content (θ_i), residual water content (θ_r), root depth (d_r) and soil column depth (d_{sc}). The sensitivity of the model in predicting both peak discharge and total discharge volume is determined for each of the four runoff producing events.

Table VII shows the sensitivity of model predictions in terms of peak discharge and discharge volume for the 0·2 and 2·0 cm cell size models, respectively. Columns two through to five list the normalized sensitivities of event peaks, with events listed in order of decreasing magnitude. See Figure 3. Column six contains the average values of columns two through five. Columns seven through eleven contain the normalized sensitivities for discharge volume. The last column, 12, contains the sensitivity of the total simulation discharge volume. Results are presented as the fractional change in model prediction for an equivalent fractional change in parameter value. A ±25% change in parameter value corresponds to a range in parameter values of 50%, and the normalized change in predicted value is

$$\Delta P_N = \frac{P_{+25} - P_{-25}}{P_0} \tag{2}$$

where P_{+25} is the predicted value resulting from a 25% increase in parameter value, P_{-25} is the predicted value resulting from a 25% decrease in parameter value, P_0 is the predicted value obtained with the original parameter value and ΔP_N is the normalized change in predicted value shown in Table VII. Equation (2) is a meaningful measure of sensitivity only when values of P_{+25} and P_{-25} are of opposite sign, or of insignificant magnitude, which is the case in this study.

Table VII. Sensitivity of the GSSHA model output to input parameter estimates, for different resolutions (0·2 cm and 2·0 cm) at GCEW. Events are listed in order of decreasing magnitude.

Resolution		Normalized parameter sensitivity										
		Event peak discharge					Event discharge volume					Volume total
		1	4	2	3	Avg	1	4	2	3	Avg	
GCEW	K_s	0·71	0·95	1·21	1·77	1·16	0·71	0·88	1·28	1·45	1·08	0·94
fine	ψ_b	0·60	0·81	1·05	1·67	1·03	0·59	0·73	0·98	1·35	0·91	0·77
resolution	λ	0·05	0·36	0·77	3·51	1·17	0·07	0·31	0·35	2·08	0·70	0·38
(0·2 cm)	e	0·63	0·72	0·87	0·08	0·58	0·60	0·64	0·88	0·24	0·58	0·60
	θ_{wp}	0·03	0·25	0·46	3·18	0·98	0·02	0·25	0·13	1·97	0·58	0·26
	θ_r	0·02	0·05	0·12	0·56	0·19	0·02	0·04	0·07	0·36	0·12	0·07
	θ_i	0·07	0·02	0·00	0·08	0·04	0·16	0·02	0·09	0·03	0·05	0·09
	d_{sc}	0·03	0·05	0·05	0·35	0·11	0·03	0·03	0·01	0·20	0·03	0·06
	d_r	0·03	0·09	0·23	2·05	0·60	0·01	0·09	0·04	1·14	0·12	0·29
GCEW	K_s	0·04	0·09	0·09	0·22	0·11	0·24	0·29	0·39	0·35	0·32	0·31
coarse	ψ_b	0·05	0·11	0·10	0·26	0·13	0·22	0·28	0·35	0·37	0·30	0·29
resolution	λ	0·09	0·12	0·14	0·39	0·18	0·54	0·47	0·72	0·68	0·60	0·61
(2·0 cm)	e	0·04	0·18	0·10	0·06	0·17	0·11	0·28	0·25	0·38	0·26	0·25
	θ_{wp}	0·02	0·15	0·07	0·37	0·15	0·10	0·36	0·33	0·47	0·31	0·29
	θ_r	0·03	0·04	0·03	0·15	0·06	0·14	0·16	0·21	0·23	0·19	0·19
	θ_i	0·25	0·11	0·26	0·49	0·28	1·02	0·53	1·13	0·99	0·92	0·95
	d_{sc}	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00	0·00
	d_r	0·01	0·09	0·06	0·21	0·09	0·06	0·22	0·21	0·30	0·20	0·18

K_s, soil saturated hydraulic conductivity; ψ_b, bubbling pressure; λ, soil distribution index; e, soil porosity; θ_{wp}, soil wilting point; θ_r, residual water content; θ_i, initial water content; d_{sc}, depth of the soil column; d_r, root zone depth.

Table 7 shows that when an adequate discretization is used, model predictions on this Hortonian basin are most sensitive to the value of the soil K_s. The next most important parameters are ψ_b, λ and e. The model is only slightly to moderately sensitive to the values of θ_{wp}, and insensitive to θ_r and θ_i. Except for θ_i, the sensitivity of model predictions to parameter values tends to diminish as the event size increases. Predictions for the smallest event, event 3, are sensitive to more parameters. Unlike during other events, model performance for event 3 is very sensitive to the value of the θ_{wp}, λ and d_r. Predictions are practically insensitive to the depth of the soil column, d_{sc}.

Table 7 also shows that when the discretization is 2·0 cm, model predictions are disproportionately sensitive to the initial moisture estimate of the soils. In fact, only the parameters θ_i and λ have a moderate to high effect on model output. Both of these parameters have a large influence on discharge volume. For these two parameters the sensitivity during individual events is dependent on order of occurrence, and not on event size, as is the case for the 0·2 cm discretization. Sensitivity to θ_i and λ tends to decrease for later storm events. For the other parameters, sensitivity tends to follow the same trend as for the 0·2 cm discretization, decreasing as event size increases. As with the fine resolution case, the depth of the soil column is a negligible factor.

At Muddy Brook the model using the G&A method to compute $K_{1/2}$, with soil layers discretized into 1·0, 2·0 and 5·0 cm cells for the first, second and third layers, respectively, is used to analyse model sensitivity. The thickness of layers varies between soil types, but the top layer is at least 10·0 cm thick in all cases. Unsaturated cells below the third layer and above the specified groundwater boundary are 10·0 cm. The number of computational points in the unsaturated zone is 55 640.

At Muddy Brook most of the stream flow is derived from base flow. Surface runoff is only significant during one large event (Figure 4). During the study period, peak discharges are very small, $< 0.17\ m^3\ s^{-1}$ for all events. The sensitivity of model predictions to parameter values for the Muddy Brook watershed is shown in Table VIII. The soils at the Muddy Brook watershed are much coarser than at GCEW, and discharge from the watershed is generated primarily from groundwater discharge to the stream and from saturated source area runoff, with a very small contribution from the infiltration-excess mechanism. This is reflected in the sensitivity analysis. Total discharge volume is most sensitive to the value of e because e is important in the occurrence of saturated source areas. The porosity also has the greatest effect on the peak discharge, which affects both Hortonian runoff and the formation of saturated source areas.

Spatial convergence with fluctuating water table

The spatial convergence with the Muddy Brook model is repeated with the fluctuating water table added to the model described for the sensitivity analysis. Over the simulation period the water table varies approximately

Table VIII. Normalized parameter sensitivity for Muddy Brook watershed

	Peaks	Volumes	
	Event average	Event average	Total
K_s	0·62	0·44	0·18
ψ_b	0·76	0·58	0·26
λ	0·56	0·48	0·34
e	1·02	0·56	0·46
θ_{wp}	0·16	0·16	0·14
θ_r	0·06	0·19	0·19
d_r	0·24	0·26	0·22

K_s, soil saturated hydraulic conductivity; ψ_b, bubbling pressure; λ, soil distribution index; e, soil porosity; θ_{wp}, soil wilting point; θ_r, residual water content; d_r, root zone depth.

1·0 m at wells near the stream (Downer, 2002). For this test, only the surface-layer cell size is varied. Results for total infiltration, runoff and ET are shown in Figure 9. The system response with a fluctuating water table is very similar to the response for a fixed water table, Figure 5. Using the G&A method to compute $K_{1/2}$ at the soil surface allows a cell size of 2·0 cm to be used with little deviation from the solution with the finest discretization (Figure 9). With upper layer discretizations >2·0 cm, the results deviate substantially from the solution. Although the decrease in total infiltration with increasing cell size is generally small, even with 50·0 cm cell sizes, the resulting increases in runoff and outlet discharge are large because so little of the precipitation becomes surface runoff. Figure 10 shows the response of different sources of outlet discharge to increasing cell size. Total discharge and groundwater discharge to the stream increase with increasing cell size over the range of cell sizes studied. Surface runoff increases until the cell size reaches 10·0 cm, then no surface runoff is generated owing to the increased infiltration using the G&A method. Exfiltration increases until the cell size reaches 25·0 cm and then begins to decrease. At cell sizes of 25·0 cm and larger the increased groundwater discharge to the stream has the effect of lowering the water table enough to reduce exfiltration.

Final calibration

With the proper RE discretizations determined at each site, model calibration can be completed. Parameters in each model are calibrated based of the results on the sensitivity analysis. In addition to a uniform value of channel roughness (n_{chan}), nine parameter types were adjusted as described by Downer and Ogden (2003a) for the nine STLU classes at GCEW:θ_i, K_s, ψ_b, e, λ, θ_{wp}, θ_r, overland flow roughness coefficient (n_{ov}) and retention depth (d_{ret}). At Muddy Brook, additional uniform parameters, saturated media lateral hydraulic conductivity (K_{gw}), saturated media porosity (e_{gw}), hydraulic conductivity of the river bed material (K_{rb}), thickness of the river bed material (M_{rb}) and maximum root depth (d_r), were also adjusted for calibration with a moving water table, as described by Downer, 2002).

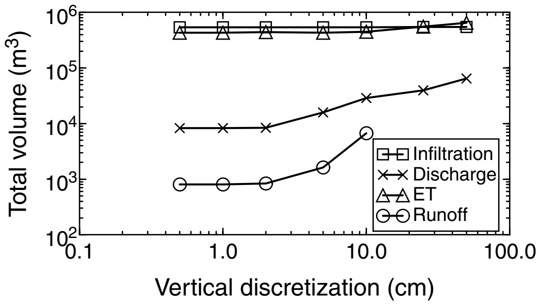

Figure 9. Spatial convergence at Muddy Brook when using a fluctuating water table as the lower boundary condition for RE solution

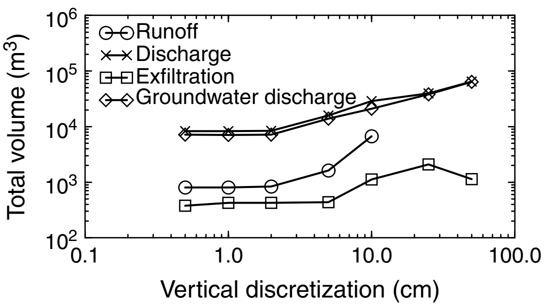

Figure 10. Stream flow contributions at Muddy Brook when using a fluctuating water table as the lower boundary condition for RE solution

Parameter sets were selected by minimizing a cost function, computed based on event peaks and discharge volumes. The weights on peaks and volumes were equal. The weight on individual peaks was determined by dividing the peak discharge of each event by the summation of the event peaks. The weight on individual volumes was determined by dividing each peak by the total discharge respectively. This scheme places more

Table IX. Final calibrated parameter values used in RE models

Watershed	Soil[a]	Layer[b]	Depth (cm)	Δz (cm)	K_s (cm h^{-1})	ψ_b (cm)	λ	e	θ_{wp}	θ_r
GCEW	SL For	1	10	0·5	0·06	24·1	0·30	0·47	0·13	0·014
		2	30	1·0	0·06	24·1	0·30	0·47	0·13	0·014
		3	60	2·0	0·06	24·1	0·30	0·47	0·13	0·014
	SL Pas	1	10	0·5	0·12	24·1	0·30	0·47	0·13	0·014
		2	30	1·0	0·12	24·1	0·30	0·47	0·13	0·014
		3	60	2·0	0·12	24·1	0·30	0·47	0·13	0·014
	SL Crop	1	10	0·5	0·10	24·1	0·30	0·47	0·13	0·014
		2	30	1·0	0·10	24·1	0·30	0·47	0·13	0·014
		3	60	2·0	0·10	24·1	0·30	0·47	0·13	0·014
	SL Gully	1	10	0·5	0·44	24·1	0·30	0·47	0·13	0·014
		2	30	1·0	0·44	24·1	0·30	0·47	0·13	0·014
		3	60	2·0	0·44	24·1	0·30	0·47	0·13	0·014
	SAL	1	10	0·5	1·02	7·1	0·87	0·42	0·03	0·018
		2	30	1·0	1·02	7·1	0·87	0·42	0·03	0·018
		3	60	2·0	1·02	7·1	0·87	0·42	0·03	0·018
	CL For	1	10	0·5	0·25	30·2	0·30	0·45	0·19	0·07
		2	30	1·0	0·25	30·2	0·30	0·45	0·19	0·07
		3	60	2·0	0·25	30·2	0·30	0·45	0·19	0·07
	CL Pas	1	10	0·5	0·29	30·2	0·30	0·45	0·19	0·07
		2	30	1·0	0·29	30·2	0·30	0·45	0·19	0·07
		3	60	2·0	0·29	30·2	0·30	0·45	0·19	0·07
	CL Crop	1	10	0·5	0·09	30·2	0·30	0·45	0·19	0·07
		2	30	1·0	0·09	30·2	0·30	0·45	0·19	0·07
		3	60	2·0	0·09	30·2	0·30	0·45	0·19	0·07
Muddy Brook	SL Crop	1	10	1·0	0·45	27·5	0·23	0·42	0·13	0·02
		2	60	2·0	0·45	27·5	0·23	0·42	0·13	0·02
		3	30	5·0	0·45	27·5	0·23	0·42	0·13	0·02
		B	0–600	20·0	0·45	27·5	0·23	0·42	0·13	0·02
	SL	1	10	1·0	0·57	27·5	0·23	0·42	0·13	0·02
		2	60	2·0	0·57	27·5	0·23	0·42	0·13	0·02
		3	30	5·0	0·57	27·5	0·23	0·42	0·13	0·02
		B	0–600	20·0	0·57	27·5	0·23	0·42	0·13	0·02
	SAL Crop	1	10	1·0	1·50	54·2	0·39	0·42	0·10	0·04
		2	34	2·0	1·50	54·2	0·39	0·42	0·10	0·04
		3	50	5·0	1·50	54·2	0·39	0·42	0·10	0·04
		B	0–600	20·0	1·50	54·2	0·39	0·42	0·10	0·04
	SAL	1	10	1·0	1·89	54·2	0·39	0·42	0·10	0·04
		2	34	2·0	1·89	54·2	0·39	0·42	0·10	0·04
		3	50	5·0	1·89	54·2	0·39	0·42	0·10	0·04
		B	0–600	20·0	1·89	54·2	0·39	0·42	0·10	0·04

[a] SL, silt loam; SAL, sand loam; For, forest; Pas, pasture.
K_s, soil saturated hydraulic conductivity; ψ_b, bubbling pressure; λ, soil distribution index; e, soil porosity; θ_{wp}, soil wilting point; θ_r, residual water content.
[b] B (bottom) layer refers to the layer between the soil column specified with layers 1, 2, and 3, and the groundwater table. This layer is not used at GCEW because the lower boundary is a no change in flux boundary. At Muddy Brook this layer varies in size from approximately 0·00 to 6 m, depending on time and location in watershed.

Table X. Final non-RE model parameter values

Parameter	Muddy Brook					GCEW				
	Uniform	Land uses				Uniform	Land uses			
		For	Pas	Crop	Res		Gully	Pas	Crop	For
d_r (m)		0·34	0·25	0·34	0·10		0·10	0·10	0·58	0·58
vh (m)		10·00	0·25	0·50	0·10		0·10	0·10	1·00	10·00
a		0·20	0·21	0·25	0·15		0·23	0·20	0·20	0·14
C_t (s m^{-1})		0·15	0·20	0·50	0·75		0·80	0·68	0·36	0·10
R_c		120	250	20	50		200	100	17	120
d_{ret} (mm)		0·00	0·00	0·00	0·00		2·26	1·39	1·34	1·55
n_{ov}		0·08	0·08	0·04	0·02		0·38	0·28	0·30	0·23
n_{chan}	0·0371					0.0271				
K_{gw} (cm hr^{-1})	16·25					NA				
e_{gw}	0·4					NA				
K_{rb} (cm hr^{-1})	0·25					NA				
M_{rb} (cm)	0·1					NA				

For, forest; Pas, pasture; Res, residential; vh, vegetation height; a, albedo; C_t, canopy transmission coefficient; R_c, canopy resistance; n_{ov}, overland flow Manning roughness coefficient; n_{chan}, channel Manning roughness coefficient; K_{gw}, hydraulic conductivity of the groundwater; e_{gw}, porosity of the saturated groundwater material; K_{rb}, hydraulic conductivity of the river bed material; M_{rb}, river bed material thickness.

weight on larger events. Parameter values are adjusted with an automated calibration process using the shuffled complex evolution (SCE) method (Duan *et al*., 1992). The discretizations used in the final models is shown in Table IX. The observed and simulated hydrographs during the test period are shown in Figures 3 and 4. Final parameter values for both watersheds are presented in Tables IX and X. Overall mass balance for the calibration period with the models described in Tables IX and X are 0·004% and 0·19% for GCEW and Muddy Brook, respectively. The maximum event RE mass balance error is 0·0025% and 0·019% at GCEW and Muddy Brook, respectively. Event RE mass balance errors are typically on the order of 10^{-4} per cent at both watersheds.

DISCUSSION

These results indicate that when applying the RE within a distributed hydrological modelling framework to simulate hydrological fluxes at the watershed scale, the predicted fluxes converge upon a solution as the vertical discretization in the unsaturated zone becomes finer. The results also indicate that the vertical discretization used in a one-dimensional RE to simulate hydrological processes at the watershed scale can have a large influence on the volumes of hydrological fluxes computed for a series of runoff events. Varying the discretization over a range of three orders of magnitude with fixed parameter values produces estimates of infiltration that vary by nearly 2000 per cent. Although the results indicate that using a sufficiently fine discretization near the soil surface is critical, using fine discretizations deep in the soil column achieves little benefit. In simulations of the Hortonian GCEW, a surface layer with small cell sizes extending to a depth of only 10 cm produces the same results as extending the fine resolution of the surface layer down to a depth of 100 cm. In this watershed a surface layer with fine resolution of only 1 cm results in only a 2% variation from a simulation with fine discretization throughout the entire 1 m of soil simulated.

The vertical discretization also has a large influence on the sensitivity of the model to parameter estimates. The GCEW model with larger discretization (2·0 cm) is much too sensitive to the estimate of initial moisture compared with the sensitivity when using a proper discretization. With this larger discretization the influence of the initial moisture affects simulation results for the entire 61-day simulation period. When model predictions are dependent on the initial moisture estimate, the determination of appropriate parameter values is very difficult (Senarath *et al*., 2000), and resulting parameters may have physically unrealistic values. In contrast, when the proper discretization, 0·2 cm, as determined by the convergence study, is used, the value of initial moisture has almost no effect on simulation results. As this analysis indicates, when sufficiently fine discretizations are used, the model is completely insensitive to the initial soil moisture conditions. This is an important asset of the model formulation because low-uncertainty initial moisture conditions are seldom known (Senarath *et al*., 2000). Given the proper meteorological inputs, the RE formulation is able to correct errors in initial moisture estimates. This advantage is lost when the discretization is too large because the model system does not properly respond to the meteorological inputs.

Selection of a method to estimate K at the surface of the soil column also influences the estimate of hydrological fluxes. Three methods were investigated, using the cell-centred value of K, assuming saturation at the cell surface for ponded conditions, and using an average of the cell centred K and K_s for ponded conditions. Although all methods produce the same answer at very fine discretizations (0·1–0·2 cm), the solutions diverge as the cell size is increased. The alternative G&A and average methods permit the use of larger cell sizes with only small differences in computed fluxes.

The discretization near the soil surface and the method used to compute K at the soil surface are important because of the highly non-linear nature of the RE. Hydraulic conductivity depends on soil moisture, and changes in the soil moisture are dependent on K. The speed at which water can infiltrate depends on the values of K in the uppermost cells. During dry conditions, K at the soil surface can be orders of magnitude less than the saturated value. How rapidly K increases at the soil surface depends on how rapidly soil moisture increases. If cell sizes are large, the small amount of water that can enter the cell owing to the low value of K has little effect on the soil moisture of the cell. In this case, K remains low, and little or no infiltration occurs before runoff and ET deplete the available water. As shown by the sensitivity analysis, even large changes in the parameter values representing soil hydraulic properties will not negate this effect. Only having the proper resolution near the soil surface allows the process of infiltration to be properly initiated. This study indicates that a very fine resolution is required near the soil surface, considerably less than 5·0 cm. This finding is in agreement with studies of hydrological fluxes computed at the field scale (van Dam and Feddes, 2000). The success of limiting the surface-layer thickness and using different methods of calculating K_r at the soil surface suggest there may be alternatives to using such a fine resolution.

Parameters that primarily influence the soil moisture and are most important in well-drained soil conditions, θ_{wp}, θ_r and d_r, are not nearly as important at Muddy Brook as they are for GCEW because the shallow water table at Muddy Brook keeps the soil moisture high during the entire simulation. The values of ψ_b and λ are more important in the case of the non-Hortonian catchment because they control the movement of water from the shallow groundwater table back into the unsaturated zone. When the water table is used as the lower boundary condition, d_{sc} and θ_i values are determined internally from the depth of the water table and are not subject to sensitivity analysis. For this reason, and unlike the GCEW case, peak discharge predictions on the non-Hortonian Muddy Brook catchment are sensitive to the value of the soil K_s, but volumes of discharge are only moderately sensitive to K_s. Because discharge volumes are very dependent on the quantity of baseflow, they are insensitive or only moderately sensitive to all unsaturated zone parameters tested.

CONCLUSIONS

The one-dimensional RE is applicable for use in computing hydrological fluxes within a distributed hydrological modelling framework provided that the proper discretization is determined through a spatial convergence study. It is critical that the soil column be represented accurately near the soil surface in Hortonian watersheds. Predictions in Hortonian catchments are not sensitive to the depth of the soil column used in the simulations. When the proper discretization is used, predictions are not overly sensitive to other difficult-to-determine parameters such as vegetation root depth, wilting point and initial soil moisture. When larger cell sizes are used sensitivity is increased owing to discretization effects. The cell size required to properly simulate fluxes near the soil surface will most likely be very small, 1·0 cm or less, but there seems to be little need in extending this fine resolution deep into the soil column. The requirement for small cell sizes near the soil surface is a function of the dependence of K on θ and θ on ΔZ. Large cell sizes near the surface prevent the proper simulation of the soil column.

Determining a representative K at the soil surface during surface ponding is very important. Alternatives to using the cell-centered value of the first cell allowed larger cell sizes to be used without substantial differences in predicted fluxes. When substituting K_s for $K_{1/2}$ the results diverge at larger cell sizes, indicating that this scheme may be inconsistent with RE. The other alternative method, using the geometric average of K_s and K_1 to compute $K_{1/2}$, does not demonstrate this behaviour, and is therefore recommended.

The proper discretization and the thickness of the near-surface layer depends on the application and the watershed being studied. Comparison of the simulation results from the Hortonian watershed against the non-Hortonian watershed reveals that the required discretization near the soil surface in each case is not significantly different. Although it may be possible to use much larger cell sizes in other watersheds, our results did not find significant differences between required discretizations on Hortonian and non-Hortonian watersheds.

The sensitivity study results also show that calibration of RE in hydrological models with insufficiently fine discretizations will likely result in parameter values that are physically unrealistic. It also seems unlikely that the calibrated values will result in a verifiable model calibration. Only a detailed spatial convergence study will reveal the appropriate resolution in the unsaturated zone for the problem at hand.

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