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1. MODEL DESCRIPTION

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Abstract

A computer model which simulates the water balance and plant growth across three-dimensional catchments is presented. The model is a distributed parameter, dynamic eco-hydrological model called Topog_IRM. By combining physical and physiological approaches, it is well suited to investigations into landscape response to changes in the physical and biological character of the system. Model structure and algorithms are described, including model assumptions and constraints. Data requirements are specified, including options for different soil models and the generation of climate data.

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TOPOG_IRM: MODEL DESCRIPTION

1. Introduction

1.1 What is Topog_IRM?

Topog_IRM is a computer model which simulates the spatial and temporal water balances and plant growth across three-dimensional catchments. Technically it is a eco-hydrological model which uses distributed parameters to characterise landscapes. Insofar as possible or practical, Topog_IRM takes physical and physiological approaches to model hydrological and plant processes. The model incorporates interactions with soil, climate and topography. Thus, the model is well-suited to investigations into catchment response to changes in land-use which affect the physical or plant characteristics of the system.

Whilst Topog_IRM can be considered a complex process model, there are necessary abstractions and assumptions built into it which affect its precision and realism. In theory, Topog_IRM can be applied to any landscape for which the abstractions and underlying assumptions are appropriate. This is a great advantage over empirical models with only local application. On the other hand, complex process models such as Topog_IRM necessarily require extensive, detailed characterisation of the landscape. The degree to which the abstractions in the model, and the characterisation of the landscape depart from reality will affect the model's precision. For these reasons *Bevan* [1989] has suggested that most complex process models are used in practice like empirical models. For example, if the initial predictions of the model are not in agreement with observed data, model parameters are adjusted to give a better fit. Topog_IRM may be used in this fashion, but the user must evaluate the perils in doing so, and to what degree the results must be treated with caution. The most useful application of Topog_IRM lies in testing the sensitivity of a landscape to changes in one or more of its parameters. For instance, how will water yield of a given catchment change if converted from an annual pasture to a pine plantation? How would we expect the spatial variability of leaf area index across the catchment to vary as we change the rainfall regime?

1.2 What is Modelled

Topog_IRM models the following quantities as *spatially distributed responses or as a hillslope profile or as a single vertical column* on a daily timestep:

- canopy interception of rainfall
- lateral subsurface flow
- vertical drainage
- saturated/unsaturated vertical moisture dynamics, yielding soil water content with depth
- leaf, stem and root carbon
- surface energy balance, yielding transpiration and evaporative fluxes.

<u>1.2.1 Assumptions.</u> Topog_IRM uses a finite difference solution of the Richards equation to solve the vertical moisture dynamics. The assumptions of the Richards equation are that the soil is incompressible, non-hysteretic and isothermal, and that moisure moves in a single phase only; the latter does not preclude

adding effects of the liquid and vapour phase into a single response. Next it assumes that flow is via the soil matrix only, and not via macropores and larger preferred pathways. This constraint is somewhat offset by parameterisation of the soil model for effective one-dimensional performance over a suitable spatial scale, rather than by extrapolated point measurements. Next, the soil is assumed to be isotropic for the purposes of subsurface flow, that is, the saturated hydraulic conductivity of the soil is used in the formulation of Darcys law for lateral movement. Finally, we assume that the watertable depth is constant over each landscape element, and that it is parallel to the soil surface.

Plant growth is assumed to be a function of light, water and nutrients only. Light is modified by air temperature, water is modified by salt content in the root zone, and nutrients are a lumped effect of all nutritional requirements. These resources are assumed to affect carbon assimilation, and therefore growth rate, as expressed by multifactor saturation rate kinetics theory (IRM of *Wu et al.* [1993]).

Topog_IRM currently does not model:

- explicit interactions between the shallow watertable and deep aquifer systems. Work is being done to make this linkage
- hysteretic effects on matrix flow
- explicit large preferred pathways of water through soil
- unsaturated lateral flow
- advection in the surface energy balance
- plant production of reproductive material (*ie.* crop grain yield).

1.3 The Daily Timestep and Its Implications

Topog_IRM uses an explicit timestep of one day, which has implications for the way processes are modelled and the constants required. For example, we can only have a single sign of flux at the surface in a single timestep - either rainfall or evaporation. So with daily rainfall totals, we assume that it falls for the whole day at a uniform intensity. Similarly, surface evaporation is assumed to be at a steady rate over the entire timestep.

The use of daily rainfall totals has an impact on the vegetation constant 'rainfall interception coefficient'. Because rain normally occurs in bursts, and a plant canopy can intercept a given amount of rainfall for each burst, the actual interception coefficient in a daily model must be greater than that for an individual event model.

The daily timestep has implications for the surface energy balance. The surface is characterised by the Penman-Monteith equation, and net heat storage terms are assumed to be zero over the day. The energy balance for each element is considered to be independent of its neighbours; advection is ignored. Further, there is no feedback from vegetation to the driving climatic variable within a timestep. For example, the vapour pressure deficit above a closed canopy, and relevant to the atmospheric demand on the canopy, will probably be greater than the vapour pressure deficit between the soil surface and the canopy, relevant to the atmospheric demand on the soil surface.

1.4 Topog_IRM and the Topog Series

Topog_IRM is a dynamic water and vegetation simulation model that fits within the Topog series. It uses all the same procedures outlined in the Topog User Guide for description of topography and distribution of input parameters. It is not convenient to run Topog_IRM without this supporting software.

2. Data Inputs

Topog_IRM requires input parameters which fall into four broad categories - catchment description, climatic data, soils information and vegetation information. Each of these categories will be discussed in detail.

2.1 Catchment Description

The heart of the Topog System is a description of a three-dimensional land surface in terms of one-dimensional flow elements. The data input requirements and procedures for a Topog terrain analysis is described in the Topog User Guide. As such, only a brief description of the steps is given here.

The steps in a typical Topog terrain analysis are:

- collect elevation data of the catchment, comprising spot heights and/or contours
- translate the information into a format for input to SPLIN2H, *Hutchinson* [1988]
- interpolate a surface from the input data using SPLIN2H
- derive contours from the surface
- fill in missing high point and saddle data
- construct a boundary file, and if required, internal watershed and stream heads files
- perform the Topog terrain analysis.

This final step provides the catchment description files necessary to run all steady-state and dynamic models in the Topog series. They also form the basis for distributing parameters by the use of polygonal overlays.

2.2 Climatic Data

Each one-day timestep requires environmental input parameters in the form of climatic information. The data required by Topog_IRM to perform the surface energy balance and set fluxes at the surface and within the soil column are:

- year day, for radiation attenuation and daylength calculation
- maximum and minimum daily air temperature, in degrees celcius (*°C*), for light availability modification, plant respiration, evaporation and transpiration calculations

- average daylight vapour pressure deficit, in millibars (*mb*), for leaf conductance, evaporation and transpiration calculations
- total rainfall, in metres (*m*), for interception and surface flux calculations
- direct and diffuse shortwave radiation on the horizontal, in kilojules per square metre per day ($kJ/m^2/d$), for energy available to the canopy and soil surface in evaporation and transpiration calculations. They are required separately because the components are attenuated differently to a sloping plane.

In addition to the basic climatic sequence, we need a file of coefficients that modify total radiation to that incident on a plane with discrete slope and aspect. This file is unique for a given latitude, and is normally created when a climate file is generated.

Climate files are normally generated from data logged at a meteorological station. If the complete set of data is available from local measurements, then these may be input directly into the model. Alternatively, a file containing yearday, maximum and minimum daily temperature, and rainfall may be used as input to a program called Topog_CLIMATE, which is a modification of the program MTCLIM by *Running et al.* [1987]. The program uses geometric arguments to calculate extraterrestrial radiation on a horizontal surface for a given day of the year at a specified latitude. Atmospheric transmissivity is estimated by the empirical method of *Bristow and Campbell* [1984], and used to reduce shortwave radiation throught the atmosphere, and to partition it into direct and diffuse components. The daily vapour pressure deficit is calculated from maximum and minimum temperature, or maximum and dewpoint temperature if it is available. The program allows the user to extrapolate data to a study catchment at a different elevation and annual rainfall from the meteorological station.

2.3 Soils Information

Of all the required input parameters, soils data is perhaps most onerous. The solution of the Richards equation requires a soil to be described by a moisture characteristic, a relationship of water potential against water content, and a conductivity curve (a relationship of unsaturated hydraulic conductivity against either water potential or content). Such data are generally difficult and time consuming to collect.

The program that generates files of the soil moisture and conductivity curves is called Topog_SOIL. It does offer the user some choice as to the soil model they wish to use. Options are:

- *Broadbridge and White* [1988] soil model
- *Clapp and Hornberger* [1978] soil model
- *Campbell* [1974] soil model
- *Ross et al.* [1991] soil model.

2.3.1 *Broadbridge and White* [1988] soil model. This soil model was the one used during development of the Richards equation solution used in Topog dynamic models (Topog_yield and Topog_IRM). It has five (5) parameters which are measured *in situ* or by gravimetric methods. Its parameters are:

- K_s, saturated hydraulic conductivity (*m/d*)

- θ_s, saturated volumetric water content (m^3/m^3)
- θ_r, airdry volumetric water content in (m^3/m^3)
- λ_c, capillary length scale (m), a function of sorptivity
- C, a shape parameter related to structure, normally between *1.01* and *1.5*.

The Broadbridge-White soil model does not require laboratory measurement of a soil moisture characteristic, since it imposes the shape of the curves based on the parameters. It was developed from a perspective that soil water diffusivity must remain positive and finite. Relationships for ψ, θ and K were produced under this constraint. Diffusivity tends toward a finite positive value as $\psi \rightarrow -\infty$, and toward a large positive value as ψ enters the saturated region. This is sensible behaviour both physically and numerically. Further this soil model is subject to two levels of dimensionless scaling that have allowed generation of a rule for guaranteed numerical convergence in the most difficult infiltration case: high rate rainfall into very dry soil. The rule is "the widest spacing of nodes is λ_c".

K_s, θ_s and θ_r are measured easily. λ_c is a function of sorptivity which can be estimated when performing the K_s experiment. C can be estimated by experiments, as outlined in *White and Broadbridge* [1988].

2.3.2 *Clapp and Hornberger* [1978] soil model. This soil model addresses the traditional difficulty with the Campbell soil model (section 2.3.3) of hitting saturation before $\psi=0$. It also decouples the relationship between the exponents of the $\psi(\theta)$ and $K(\psi)$ curves. Its parameters are:

- b, slope of the $\psi(\theta)$ graph on a log-log plot
- n, slope of the $K(\psi)$ graph on a log-log plot
- ψ_e, water potential at air-entry point (m)
- ψ_i, water potential of inflection for quadratic smoothing of $\psi(\theta)$ curve in metres (m)
- θ_s, saturated volumetric water content (m^3/m^3)
- K_s, saturated hydraulic conductivity (m/d).

To get the parameters b and n, the soil moisture and conductivity characteristics must be measured in a laboratory. ψ_e can be estimated when measuring the $\psi(\theta)$ relationship, but ψ_i is generally a guess. θ_s and K_s can be measured easily in the laboratory when measuring the respective characteristic curves.

2.3.3 *Campbell* [1974] soil model. This soil model is simply curve fitting to experimentally derived curves for $\psi(\theta)$ and $K(\psi)$. It assumes that the slopes of the curves of $\psi(\theta)$ and $K(\psi)$ are related, and that saturation values of θ and K are reached before $\psi=0$. Its parameters are:

- b, slope of the $\psi(\theta)$ graph on a log-log plot, and $n=2+b/3$ is the slope of the $K(\psi)$ graph
- ψ_e, water potential at air entry in metres (m), the point where saturated values of θ and K begin
- θ_s, saturated volumetric water content (m^3/m^3)
- K_s, saturated hydraulic conductivity (m/d).

The main problem with this method is that it is almost impossible to accurately measure the curves close to saturation and when very dry. This means that these very important areas are extrapolated from the data in the central part of the curve that can be measured. Extrapolation is always dangerous! Specifically, diffusivity tends to zero as $\psi \rightarrow -\infty$, and diffusivity tends to ∞ as $\psi \rightarrow 0$. The very dry condition has led to infiltration into dry soil being traditionally very difficult.

2.3.4 *Ross et al.* [1991] soil model. This soil model is another attempt to overcome some of the problems with the Campbell soil model (section 2.3.3), specifically the problems when ψ is very negative. Its parameters are:

- a_2, a soil characterisation parameter
- c_2, a soil characterisation parameter
- ψ_o, water potential at over dryness (m)
- ψ_e, water potential at air entry (m)
- θ_s, saturated volumetric water content (m^3/m^3)
- K_s, saturated hydraulic conductivity (m/d).

Note that the Campbell model, and its variants, do not possess the scaling properties of the Broadbridge-White soil model that allow us to generate rules for guaranteed numerical convergence. Moreover under saturated conditions, the scheme will capriciously fail with a singular matrix. Their use should be with this in mind.

2.3.5 Soil Profile Files. Every different soil type in a catchment requires a soil table. Every different soil profile requires a Soil Profile file. This consists of a list of depth nodes for the Richards equation solution, and a soil type for each depth node.

It is very important to be clear at this stage the difference between a soil type and a soil profile. A soil profile for a duplex soil would contain two soil types, one for the upper and one for the lower layer. There must be at least as many soil types as soil profiles. A soil profile is a vertical slice describing where each soil type is located.

Each soil profile file, which associates soil types with soil layers, must be manually generated. When soils are specified in dynamic Topog models, *soil profiles* are distributed, not soil types. Each soil profile should start with some closely spaced depth nodes for modelling evaporation accurately (see sections 4.5 and 4.5.2.5 for more details), then double the node spacing until the maximum depth spacing is reached. That maximum spacing is then continued to the bottom of the first layer. The close depth nodes are not required at the top of lower layers. For these layers a uniform depth node spacing is used.

An example parameterisation of a catchment for soils follows. In this example, there are only two discrete soil profiles - one is about *0.5m* of coarse sandy-loam over *1.5m* of clay which appears on the ridges and midslopes, and the other is *1m* of fine alluvial material over *2m* of clay which appears in the valleys. Assume the Broadbridge-White soil model is applicable for these soils with the following parameters,

- soil type 1 = coarse sandy-loam: $K_s=1.25\ m/d$, $\theta_s=0.4$, $\theta_r=0.1$, $\lambda_c=0.1m$, $C=1.4$,
- soil type 2 = base clay: $K_s=0.05\ m/d$, $\theta_s=0.5$, $\theta_r=0.3$, $\lambda_c=0.5m$, $C=1.02$,
- soil type 3 = alluvium: $K_s=0.25\ m/d$, $\theta_s=0.45$, $\theta_r=0.2$, $\lambda_c=0.2m$, $C=1.1$.

There are two soil profile files

soil profile 1

depth (*m*)	soil type
0.0	1
0.0005	1
0.001	1
0.002	1
0.005	1
0.01	1
0.02	1
0.05	1
0.1	1
0.2	1
0.3	1
0.4	1
0.5	2
1.0	2
1.5	2
2.0	2

soil profile 2

depth (*m*)	soil type
0.0	3
0.001	3
0.002	3
0.005	3
0.01	3
0.02	3
0.05	3
0.1	3
0.2	3
0.4	3
0.6	3
0.8	3
1.0	2
1.5	2
2.0	2
2.5	2
3.0	2

Notice how they have different lengths? They have different spacings in the layers (see section 2.3.1). Notice that soil profile 1 contains soil types 1 and 2, and soil profile 2 contains soil types 3 and 2. Notice also that the soil type changes at the depth node which is equal to the layer boundary. When distributing soil profiles, the number of the file corresponds to the order they are entered into Topog_IRM. Changing the order of the files changes the soil types and/or the soil profiles assigned to each element. The same principle applies with distributing vegetation types.

2.3.6 Initial Catchment ψ. Every simulation requires an antecedant condition. This is specified in Topog_IRM as either a constant ψ over the whole catchment, or the final condition of another run of the model.

Using an initially uniform ψ can be very inaccurate, except probably in summer after all lateral flow has ceased, the catchment has dried out, and the initial condition is very dry. If a catchment starts from a wet initial condition, it may take some time for the ridges to drain reasonably into the valleys, and a realistic distribution of soil moisture to develop.

Using the final condition from a previous run will certainly get a more realistic distribution of moisture initially, but there is no point starting a simulation in summer from the catchment condition in winter! The antecedant condition of a catchment remains a difficult state to measure and impose, but for a long term daily timestep model such as Topog_IRM, its effect is generally short term only.

2.4 Vegetation Information

The dynamic vegetation response and growth modelling in Topog_IRM sets it apart from other dynamic Topog System models. Unfortunately, it also requires many parameters for the physiological models of vegetation interaction with the surface energy and water balances. The benefit is that it gives the user many more questions to address with respect to land management, and initial conditions and the state of the vegetation environment.

<u>2.4.1 Vegetation Coefficients File</u>. Topog_IRM requires a file that contains each of the twenty-two (22) parameters for each vegetation type. Each of the parameters will be described, its units, normal range and special values stated, if applicable. Parameters in the vegetation coefficients file are:

- 1.0 minus albedo of the canopy (dimensionless in the range [0,1]) is used to determine how much radiation is available to the canopy (and ultimately to the ground surface)
- 1.0 minus albedo of the soil (dimensionless in the range [0,1]) is used to determine how much light that has passed through the canopy is available for evaporation
- rainfall interception coefficient (*m/LAI/d*, must be greater than zero) is used to calculate how much rainfall reaches the ground surface
- light extinction coefficient (dimensionless, must be less than zero) is used in Beers Law to determine how much radiation is captured by the canopy
- maximum assimilation rate (*μmoles/m^2/s*, must be greater than zero) is modified by growth rate to determine how much carbon is assimilated each timestep
- slope parameter of *Ball et al.* [1987] stomatal conductance model (must be greater than zero) is used to calculate canopy conductance for Penman-Monteith
- maximum plant available soil water potential (*m*, must be wetter than the driest potential on every soil table) is used to scale water availability to the plant
- IRM weighting of water relative to light (dimensionless, must be positive) is used in the IRM equation to calculate growth rate
- IRM weighting of nutrients relative to light (dimensionless, must be positive) is used in the IRM equation to calculate growth rate
- temperature when growth rate is ½ of optimum (*°C*) is used to modify the availability of light with the average air temperature
- temperature when growth is optimum (*°C*) is used to modify the availability of light with the average air temperature

- yearday of plant germination (in range [1,365]) is used to initialise growth of annuals; set to -1 if the vegetation is perennial
- degree-daylight hours of growing season (*°C·hr*, must be greater than zero) is used to impose senescence on annuals; set to -1 if the vegetation is perennial
- saturation light intensity (*μmoles/m²/d*, must be greater than zero) is used to scale the availability of light
- maximum rooting depth (*m*, must be greater than zero) is used to calculate rooting density function with depth for transpiration
- specific leaf area (*m²/kg C*, must be greater than zero) is used to convert leaf carbon to Leaf Area Index
- leaf respiration coefficient (*kg/kg/°C/d*, must be greater than zero) is used to calculate leaf respiration
- stem respiration coefficient (*kg/kg/°C/d*, must be greater than zero) is used to calculate stem respiration; set to -1 if plant has no woody stem
- root respiration coefficient (*kg/kg/°C/d*, must be greater than zero) is used to calculate root respiration
- leaf mortality (*% leaf C/d*, must be greater than zero) is used to calculate daily mortality of leaves
- soluble carbohydrate pool size as fraction of leaf C (dimensionless, must be greater than zero) is used to set the limit on the size of carbohydrate pool plants keep for hard times
- salt sensitivity factor (dimensionless, must be greater than zero but stays close to one) is used to modify the osmotic potential of salt in the root zone as it affects water availability.

Details of some sources for the values of these coefficients as they appear in the vegetation file of Topog_IRM can be found in *Hodges* [1992].

<u>2.4.2 Vegetation Distribution</u>. Each simulation requires a spatial distribution of vegetation. Vegetation type can be distributed, that is, the numeric value of the order of sets of vegetation coefficients in the vegetation coefficients file, as you would any other parameter. So if the coefficients for eucalypts appeared first in the file, they would be vegetation type 1. And if the coefficients for lucerne were the third set, then lucerne would be vegetation type 3. But note that only a number is distributed, and if the order of the sets of coefficients in the vegetation file change, then this will change the type of vegetation.

The other option is to make the vegetation uniform over the catchment, but again only the number of the vegetation type desired is specified.

<u>2.4.3 Initial Carbon Values</u>. For each vegetation type present on the catchment, the initial amount of carbon allocated to leaves, stems and roots must be specified. In fact, only the leaves are given an absolute carbon allocation initially; the others are calculated from ratios to leaf carbon.

Some of the values of vegetation coefficients should be noted. For example, if specific leaf area was *10.0 m²/kg* and a mature stand of vegetation with an *LAI* of *4.0* was to be specified, then the initial leaf carbon would be *0.4 kg/m²*. With ten times as much stem as leaf, the initial leaf:stem ratio would be *0.1*, and not

4.0 kg/m^2! Similarly, with twice as much root carbon as leaf carbon, initial leaf:root ratio is specified as *0.5*.

2.4.4 Growth Option. At this stage, the user can opt to not grow vegetation at all leaving LAI static, that is, no growth and no death. With static vegetation, a number of inputs are not required. Even if growth does not occur, the calculations required for IRM growth rate are performed. This is because assimilation is modelled as a feedback on canopy conductance.

2.4.5 Nutrients. Nutrients are modelled in Topog_IRM as the effect of all nutritional requirement as a zero to one scalar, representing their availability. This scalar can be distributed over the catchment in the same way as other parameters. It would be possible, if such data were available, to model nutrient availability as some function of the availabilities of individual nutritional components such as potassium, nitrogen and phosphorous. Such data is considered too difficult to collect, and interaction of nutrients is difficult to quantify and combine. It would also be possible to modify nutrient availability by soil pH, but a form of relationship for this interaction has yet to be included in Topog_IRM.

2.4.6 Salt in the Root Zone. Salt is a constant but distributable parameter for each simulation. The value assigned is the fraction of soil by weight that is salt. A value of *0.001*, or *0.1%*, is considered saline and will retard plant growth significantly. Salt dissolved in the water of the root zone exerts osmotic pressure that inhibits plant uptake of water. In this way, water can become the factor most inhibiting growth.

There is a parameter in the vegetation coefficients file called the salt sensitivity coefficient. Normal vegetation has a value of *1.0*, meaning that all the osmotic potential exerted by dissolved salt inhibits plant uptake of water. A salt tolerant vegetation may have this value reduced to *0.75*, indicating that the plant only 'feels' *75%* of the osmotic potential when extracting water. Similarly, a salt sensitive vegetation may have this value increased to *1.5*, for example.

2.4.7 Grazing. Topog_IRM allows the user to enter, or distribute, a value representing the stock equivalent units of animals grazing on the catchment. This concept only has real meaning when stock are grazing pasture, although the model has no real way of differentiating between trees and grass. As such, the user could specify stock equivalents of koalas, removing leaves from a eucalypt covered catchment. One stock equivalent unit is a wether (sheep) eating enough to hold present condition. In model terms it amounts to *0.5 kg* of leaf carbon removed per hectare per day, per stock unit.

The starting and ending yeardays for grazing must be specified, so that you only graze winter pasture in the spring and summer, for example. There is currently no temporal variation in stocking rates, other than this on/off mechanism. For setting temporal variations, such as grazing one paddock for half of the year, then another paddock for the rest of the year, you must end one simulation when the stocking changes, then restart from the final condition with new stocking conditions.

2.4.8 Generating Parameter Files. It would be very tedious and error prone to manually enter each of the required inputs each time the program Topog_IRM is run. A program exists called Topog_IRMGEN that allows users to enter the required parameters in a safe environment with online help for each question. With this utility program, a text file is created with all the required parameters in the correct order. It is then very easy to manually edit this file to make small changes to parameters.

3. Data Outputs

Topog_IRM allows the user to request two basic types of data output - time series, *ie.* one point in space followed through time, and space dumps, *ie.* one point in time shown spatially.

3.1 Time Series Data

Time series data is the type of data most often collected. It consists simply of a response variable measured at a single point in space over a period of time. Examples of this type of data are a hydrograph measured at a weir, water level in a piezometer, soil moisture from a neutron moisture meter nest, and the like.

Topog_IRM allows many variables to be recorded as time series data (called "trace" files). These are

- rainfall water balance components, including gross rainfall, interception by vegetation canopy and net rainfall onto the ground surface,
- discharge water balance components, including subsurface flow, overland flow and recharge to a deeper system,
- vegetation water balance components, including soil evaporation and plant transpiration,
- vegetation growth and carbon components, including leaf area index, leaf carbon, stem carbon, root carbon, and relative growth rate,
- the value of water content, θ, for every depth node of an element.

These data are presented in a series of four file. They are

- catchment hydrograph file containing catchment averages for rainfall, discharge and vegetation water balance components all in *mm* (*ie.* flux m^3 / catchment area $m^2 \times 1000$), as well as catchment average leaf area index,
- element hydrograph file containing all the data for the previous file, but for the specified element only,
- element vegetation trace file containing leaf area index, leaf, root and stem carbon, and relative growth rate for the element,
- element depth trace file containing the water content, θ, for each depth node of the element.

These files are plotted on a set of cartesian axes, with time on the X-axis, and the response variable on the Y-axis. A program exists that takes the files mentioned and plots them on a graphics screen using a mouse driven interface.

3.2 Spatial Data

The second basic type of data Topog_IRM can report is spatial data, that is a look at the value of a parameter that varies in space at a given time. These are perhaps the most interesting outputs from Topog_IRM, since they clearly show the distributed and connected nature of the modelling performed.

Topog_IRM allows the following variables to be recorded (called "dump" files)

- this days recharge, in *mm/day*,
- mean recharge since last dump of this type, in *mm/day*,
- cumulative recharge since last dump of this type, in *mm/day*,
- this days soil evaporation, in *mm/day*,
- this days plant transpiration, in *mm/day*,
- this days total evapotranspiration, in *mm/day*,
- this days final soil moisture state, as a table of water content with depth for every element,
- this days final double-sided leaf area index, in m^2 leaf / m^2 ground.

Each of the different data responses are recorded in a separate file with a unique file extension.

These files are generally plotted as a map with a scale of grading colours indicating the value of the response. A program exists that can easily plot the files mentioned on a graphics screen. It automatically searches for the file extensions, and it is run with a mouse driven interface.

4. Program Structure

4.1 Data Requirements

The data requirements of a physically based model will be greater than that of an empirical model. In our case of a catchment scale model, say 10^{-1} to 10^{1} km^2, with explicit physical and physiologically based models of moisture and surface energy balance, and vegetation dynamics, the minimum data requirement is large. Along with this large data requirement, goes the task of checking that data is within reasonable bounds.

An empirical model can take into account the values and interactions of any number of physical variables with a single parameter. As such, limits on the fitted value of empirical parameters may be difficult or impossible to determine. Further, as one or more of the physical variables encapsulated in an empirical parameter vary, their effect on the parameter may not be known. This has dire implications for simulations requiring that management strategies be distributed or in other ways modified. Finally, a fitted empirical parameter will often have no recognisable meaning in the real world. This can be a great problem where parameters must be estimated or guessed.

The whole task is simpler with physically based models. There are often simple limits to parameter values, *eg*. albedo must be between *0* and *1*. In addition, there may be some physical limit to parameter values, *eg*.

the maximum assimilation rate of a vegetation type is greater than *0*, but always less than *100*. When a variable changes locally, then the physical formulation accounts for the interactions with other variables and the processes modelled. Lastly, a physical parameter has a real world meaning, and can most often be directly measured, and seen or touched.

A final warning note about physically based models. Almost all physical models of a real world process or situation have a set of simplifying assumptions. When applied to problems that violate these assumptions, all results can be expected to be in error, and the errors will increase with increasing divergence from the model assumptions. So while physical parameters can be measured, and theoretically physically-based models apply to any situation where the assumptions hold, the user must beware of cases where the assumptions are violated and how applicable a model is to your particular scenario.

4.2 Data Entry and Checking

All data entry and checking is handled in a single routine within Topog_IRM called *XDATA*. This is an interrogative subroutine that prompts for each piece of infomation. It would be tedious and fraught with error to enter each required parameter each time the model is run. It is therefore common to create a file that contains the answers to the questions that can be used as input to Topog_IRM. These data files are created with a utility named Topog_IRMGEN. Both Topog_IRM and Topog_IRMGEN perform a certain amount of error checking, to be described here.

4.2.1 Error Checking in Topog_IRMGEN. The datafile generator program does not perform exhaustive error checking on each parameter and file. It does perform a minimum of checking to ensure that the minimum required parameters are in the correct order, and within the most easily defined bounds.

Topog_IRMGEN will not proceed if the basename for Topog files given does not have an **.atr** and **.cct** file associated with it. Topog_IRMGEN reads in the element connections file to determine how many contours are used, and how many elements are on each contour. These data are used when the user specifies elements to trace by hydrology, vegetation or depth, by entering a contour and element number. It also performs a simple integrity check to ensure the file has not been corrupted.

Topog_IRMGEN reads in each line of the vegetation coefficients file as dummies; the only information retained is the number of lines in the file. This is required for checking uniform vegetation type is within the acceptable bounds, or that a distributed vegetation file has all types within bounds. It reads in the necessary number of dummies per vegetation type, so it can detect if there are too few or many parameters for the last vegetation type.

Topog_IRMGEN will issue a warning for any datafile specified that it cannot find. This most often signifies a typographical error, but may indicate that the datafile is yet to be created or that it cannot be accessed for some reason.

Topog_IRMGEN is an intelligent program that asks only the questions that need to be answered. With only one vegetation type, for example, then there is no reason to ask for distributed vegetation types. Similarly for soil profile description files. And if plant growth is not modelled, then grazing cannot be modelled; leaf area must remain constant.

4.2.2 Error Checking in Topog_IRM. A massive amount of code in the subroutine *XDATA* in Topog_IRM is dedicated to the task of exhaustively error checking each input parameter and the existence and integrity of each input datafile.

Data entry and checking, in order, consists of:

- the Topog basename is checked to ensure necessary topographic analysis file are present
- the start yearday is checked to be positive, and the end yearday is checked to be greater than or equal to the start yearday
- each soil layer file is checked for a Broadbridge and White header so calculation of maximum depth node spacing can be made, lookup table parameters are calculated, file is checked to ensure that ψ values, the index variable, are monotonically increasing
- each soil profile description file is checked to make sure it specifies soil files up to the number entered, and that depth nodes are monotonically increasing in depth
- if a soil profile description distribution file is required, then the file is checked to ensure that soil profile description files up to the number entered are specified
- the three drainage terms are read in and a warning is produced if the drier multiplier is less than the wetter multiplier; this can cause the solution to oscillate
- a radiation attenuation coefficients file is read in, structure is checked implicitly by reading unconditionally
- read the vegetation file and check each parameter for reasonable bounds; most are simply *'must be greater than zero'*, but others such as albedo have a finite range
- the value of ψ where the soil becomes airdry is calculated as the average of the least negative ψ at the end of all soil tables and the most negative soil water potential that a vegetation type can extract water from
- the weather file has the first year of data read in and sums of degree-daylight hours are made for initialising the amount of growth of annuals, if the simulation starts within their growing season
- check vegetatation type if uniform for limits with number of vegetation types in the vegetation coefficients file, or check each value in a vegetation distribution file for these limits
- rooting density of each vegetation type is calculated by a negative exponential function to the minimum of the soil depth and biological maximum rooting depth
- get initial leaf carbon value, or distribution, for each vegetation type used, in kilograms, and ensure it is not negative
- get initial leaf to stem, and leaf to root ratios, or distributions, for each vegetation type used, as a scalar, and ensure they are greater than zero
- get relative nutrient availability value, or distribution, and ensure it is between zero and one

- get fraction of soil weight that is salt, or distribution, and ensure it is between zero and one
- if applicable, get grazing stock equivalents value, or distribution, and ensure that they are not negative
- if applicable, get grazing start and finish yeardays, and ensure they are between *1* and *365*
- get soil initial ψ value if uniform, and ensure it is not saturated, *ie.* less than $\psi=0$
- may require initial soil ψ distribution file, structure is checked implicitly by reading unconditionally
- for all hydrologically traced elements, ensure that input contour is within valid range, and that input element is within valid range for that contour
- for all vegetation traced elements, ensure that input contour is within valid range, and that input element is within valid range for that contour
- for all depth traced elements, ensure that input contour is within valid range, and that input element is within valid range for that contour
- for each space dump, ensure that a valid dump type is specified and that the times are not decreasing with successive dumps.

Even with the extensive level of error checking on input parameters, there is no guarantee that this model will produce results consistent with everybody's experience. To stress the main message in the Introduction again, ***as a particular site or scenario diverges from the assumptions built into the physical and physiologically based models used in Topog_IRM, so the predicted results must diverge from reality/observation***.

4.3 Water Balance Module

The Richards Equation is the heart of the Topog dynamic simulations as it is the water balance model. A finite-difference numerical solution of the Richards Equation was chosen ahead of simpler integral methods for the following reasons:

- integral methods did not have a fundamental method to handle a perched watertable
- with an appropriate form of the Richards Equation and an amenable hydraulic model they are slower
- the Richards Equation is general and based on physics, whereas integral methods are based on the simplification of moisture profiles and intuition
- sources and sinks can be introduced simply at any point in the profile as part of the Richards Equation formulation.

The solution scheme used is based on the work of *Brutsaert* [1971], recently rediscovered by *Ross and Bristow* [1990], but uses the soil hydraulic model developed by *Broadbridge and White* [1988]. This particular soil model was chosen for the following reasons:

- it can realistically represent a comprehensive range of soil moisture characteristics, from the highly nonlinear associated with a well developed capillary fringe, to the weakly nonlinear associated with highly structured soils and macropores, by varying a single parameter
- it has only five parameters; four of which are directly measurable *in situ*, and the fifth may be estimated by a simple infiltration test

- analytic solutions are available for the case of constant rate infiltration with or without an impermeable base, and with any initial moisture
- it has scaling properties that lead to a set of dimensionless variables, capable of yielding guidelines for guaranteed numerical convergence
- it has a monotonic function $\psi(\theta)$ for all $\psi<0$, and does not make the derivative zero at $\psi=0$.

<u>4.3.1 Assumptions</u>. The water balance module of Topog_IRM make the following assumptions:

- that vertical movement occurs via an isothermal, isotropic, incompressible and nonhysteretic soil matrix (this assumption is explicit in using the Richards equation)
- that water movement is in the liquid phase at all times
- that lateral flow occurs only via a saturated watertable which is parallel to the ground surface, and those fluxes are described by Darcys' Law using the surface slope
- that macropore effects can be represented as a bulk soil property, at the spatial scale of an element, within the soil hydraulic model
- that pipes and any other large preferred pathway mechanisms do not operate
- that in one timestep, currently one day, only one sign of flux operates at the surface, *ie.* either rainfall or evaporation, and that the flux is constant over that timestep
- that any water ponded on the surface appears as outflow within the timestep.

<u>4.3.2 Logic Flow</u>. The water balance routine in Topog_IRM uses the following logic flow:

- sum lateral subsurface fluxes from upslope
- determine minimum water content and hydraulic conductivity for each soil depth node
- calculate radiation attenuation value based on slope, aspect and yearday, and daylength
- CALL evapotranspiration routine
- ## re-entry point if solution fails, or otherwise needs to be restarted ##
- get values of soil water functions for the start of the timestep
- determine recharge multiplier for the timestep
- LOOP
    - get values of soil water function for current estimate for end of timestep
    - calculate coupling fluxes of subsurface flow
    - calculate coefficients for solution matrix, (adding in evaporation/rainfall, transpiration, lateral flow and recharge, and taking into account the current surface boundary condition)
    - solve the matrix equation
    - check for convergence
    - modify estimate at end of timestep, reducing oscillation and extreme jumps in value
    - estimate new watertable depth and subsurface fluxes
- check for solution failure and timestep underflow, and re-enter solution if necessary
- check for a change in surface boundary condition, and re-enter solution if necessary
- accumulate all fluxes in this timestep for mass balance
- route any subsurface fluxes downslope

A full description of, and references for, the equations used and solution method employed is found in Appendix 1 of this work. It describes the raw equations, their terms and forms, the soil water functions used during development, formulation of the finite-difference equations, the solution technique and convergence assurance.

4.4 Plant Growth Module

The plant growth model used in Topog_IRM is based in part on Integrated Rate Methodology as described by *Wu et al.* [1993]. The equations and models presented are designed to be physical or physiologically based where possible, minimizing the empirical relationships and decisions to be made.

4.4.1 Logic Flow. The growth routine in Topog_IRM uses the following logic flow:

- calculate leaf and root carbon maximums
- determine relative light and nutrient availability, and calculate temperature modifier
- calculate relative growth, *g*, according to the IRM combination equation
- initiate growth of annuals, if required, on their germination day
- accumulate degree-daylight hours for annuals, if required
- calculate gross assimilation for the day
- calculate leaf dark respiration, root and stem maintenances
- apply senescence to annuals past their DDH, by setting $g=0$ and increasing maintenance 10-fold
- convert gross assimilate to kilograms of carbon fixed, and reduce by maintenances
- calculate dynamic leaf to root partitioning ratio
- if there is an assimilate deficit, *ie*. plant cannot cover respiration
    - reduce soluble carbohydrate pool first
    - reduce leaf carbon and root carbon, according to leaf to root ratio, if any loss remains
- if there is an assimilate surplus, *ie*. growth can occur
    - fill soluble carbohydrate pool first
    - if any remains, take 2% and give to stems
    - if leaves at maximum
        - give all the rest to stems
    - otherwise
        - partition remainder to leaves and roots, according to the leaf to root ratio
    - modify additions to carbon pools by fixing efficiency
- calculate leaf, stem and root mortalities
- remove leaf carbon for grazing, if required
- update leaf, stem and root carbon pools for assimilation, respiration and maintenance.

4.4.2 Discussion. The dynamic allocation and reuse of carbon remains a poorly understood area. What factors affect how assimilate is partitioned between growing leaves, roots, stems and reproductive material? What are the relationships between carbon pools in this partitioning? What affects which parts of the plant are reclaimed when there are stresses on the plant? What are the relationships between carbon pools in this reclamation?

The mechanism for imposing senescence on annuals is crude, but probably realistic. To determine the lifespan of annuals we use the 1960s concept that an annual grows for a certain number of degree-daylight hours then dies. This model is simple and effective, but may require updating given a more appropriate indicator of annual plant lifespan.

Something that this model assumes is that plants are greedy, constantly germinate, and attempt to fully stock an area if possible, *ie*. when conditions are good, the vegetation attempts to close the canopy and develop a maximum leaf area. For systems that require an external event for germination, or that evolve into poorly stocked stands, this model will necessarily overestimate growth and carbon pools. Further if conditions dictate that the system becomes poorly stocked or even collapses, then there is only the random mechanism for suggesting that the germination event has occurred. An example of such a system are the *E. regnans* forests in the Melbourne Board of Works water supply catchments. These trees grow very large over hundreds of years, and do not replace fallen members. They require a hot fire to clear out the system and initiate germination of the next generation.

<u>4.4.3 What is not Modelled</u>. The plant modelling descibed here does not attempt to model the following,

- detrimental effects of short or long term extremes in growing conditions, *eg*. the effect of below freezing conditions on frost susceptible plants, or the long term effects of very high daytime air temperatures on leaves
- toxicity of limiting factors on growth response, *eg*. anaerobosis in saturated soil, nutrient toxicity when in high concentrations, photoinhibition, long term plant retardation or death from these or other factors
- stochastic catastrophic meteorological or physical events in a plants life, *eg*. fires, floods, insect plagues or severe storms
- individual plants and/or cohorts of leaves; the model is abstracted to pools of carbon for roots, stems and leaves representative of vegetation for each land element.

<u>4.4.4 Short Derivation of IRM</u>. The derivation of IRM stems from the Michaelis-Menten-Henri equation, *Segel* [1975], a single factor model that describes the rate of an enzymatic reaction. The multiple factor implementation, including weighting factors and modifiers of availability, has been developed by *Wu et al.* [1993].

In its basic form it is a weighted harmonic mean of any number of factors describing the relative strength, a zero to one number, of a response limited by these factors. For the application to plant growth in Topog_IRM, the response is growth rate with the following limiting factors:

- light, a function of canopy intercepted radiation, as modified by air temperature (this is the reference response for other weighting factors)

- water, a function of the soil water in the root zone, and the rooting density, as modified by the presence of salt
- generic nutrient, a constant but distributed factor.

Other responses and weighting factors that could be introduced include:

- atmospheric CO_2 concentration response, which would affect growth rate and stomatal conductance as it is currently modelled
- pH as a weighting factor for nutrient availability
- the inclusion of a full IRM equation for multiple nutrients, factors, such as nitrogen, phosphorous and potassium, and any necessary weighting factors, for the nutrient factor in the growth rate equation. Such an inclusion would demonstrate a self-similar recursive functional form.

The general form of the IRM equation is,

$$r = \frac{\sum w_i}{\sum w_i / (m_i\, f_i)}$$

where r is the response, from zero to one, w_i are the weightings of each factor, which may take any non-zero positive value, f_i are the factors on a zero to one scale, and m_i are modifiers to the factors, also on a zero to one scale. Such m_i do not necessarily exist for each factor, but the equation is general enough to allow for any combination.

This equation follows all the intuitive rules for such a combinatorial equation. They are:

- if any one of the modifiers or responses are zero, then the response r is zero
- only if all the modifiers and responses are one, can the response r be one
- with any other combination of modifiers and responses, the response r is between zero and one.

The specific equation used in Topog_IRM is,

$$g = \frac{1 + w_H + w_N}{1/(t\, L) + w_H / H + w_N / N}$$

where w_H is the weighting of water relative to light, w_N is the weighting of nutrients relative to light, L is the relative availability of light, t is the modifier to L due to temperature, H is the relative availability of water, and N is the relative availability of nutrients.

One of the satisfying aspects of this combination equation is that the weightings w_i are physiological constants for a plant species. For example, the weightings for a particular strain of wheat will remain constant regardless of where the wheat is planted. Evolution of species in different areas will necessarily have different weightings and modifiers to the limiting factors according to local conditions. This combination equation is unproven and no evidence exists to show that factors limiting plant growth combine in this, or any other, particular manner. In real terms, this is a convenient and satisfying empirical equation.

4.5 Evapotranspiration Module

The evapotranspiration model described here uses the Penman-Monteith equation, and is linked with the plant growth model. The canopy conductance is modelled according to *Ball et. al.* [1987] which requires the plants assimilation. We can only get an estimate of assimilation after going through the growth rate calculations descibed earlier, thus as part of estimating transpiration, growth must be detemined.

4.5.1 Logic Flow. The evapo-transpiration routine in Topog_IRM uses the following logic flow:

- get total incoming solar radiation, adjusted for slope and aspect of element
- calculate net longwave (*Jury and Tanner* [1975]) and subtract from radiation
- determine root water experience by multiplying soil moisture content by rooting density for every soil node within the rooting zone
- determine resistance length of the soil to evaporation
- calculate osmotic potential of water in root zone
- calculate osmotic potential of salt (*Metten* [1966]) dissolved in the root zone
- calculate relative availability of water
- calculate radiation intercepted by canopy, and that which hits the soil surface
- calculate rainfall interception, if any
- CALL growth routine
- reduce CO_2 availability for vapour pressure deficit (*Wong and Dunin* [1987])
- calculate canopy conductance (*Ball et. al.* [1987])
- generate constants and coefficients for Penman-Monteith
- if soil surface is airdry, return a fraction of soil surface radiation to the canopy as sensible heat
- set aerodynamic resistance to $r_a=50$ for crops (no stems), or $r_a=12$ for trees (with stems)
- calculate daily transpiration rate using Penman-Monteith
- calculate surface resistance (r_s) of soil from resistance length (*Choudhury and Monteith* [1988])
- calculate daily evaporation rate with Penman-Monteith, setting $r_a=100$
- distribute transpiration down soil profile according to water content and rooting density.

4.5.2 Discussion. Most of the weak links in this routine are estimations of resistance (or conductance) terms. Some of these terms are simply set as constants, others use empirical relationships, and the specification of soil depth nodes has become more important to evaporation. These resistance terms can become somewhat of a "catch all", in the sense that these terms may be adjusted to fit the observed data.

4.5.2.1 Incident Radiation. Global radiation is broken into two terms in the climate file - direct and diffuse. Each of these components is treated differently when detemining the radiation incident on an element.

The direct component is modified according to the slope and aspect of the element and time of the year. These calculations take into account self shading, but no topographic shading is calculated. Direct radaiation may be reduced to zero with some combinations of slope, aspect and time of year. The diffuse component is modified empirically by slope alone. It is reduced so that a minimum of half of this component is received.

Light availability is calculated as a linear function relative to a saturation value. No modelling of photo-inhibition is done.

4.5.2.2 Net Longwave Loss. Once total incident radiation is calculated, it is reduced by the net longwave leaving the system. This calculation is from *Jury and Tanner* [1975]. The air temperature and daylength required for this calculation are either input parameters or simple to calculate empirically, but it requires an atmospheric transmissivity term. This is set to *0.5* if it is a rainy day, and to *0.95* if there is no rain. This is an area where a simple empirical model would be useful.

4.5.2.3 Salt in the Root Zone. The relative availability of water is modified by the osmotic potential of dissolved salt. The salt content of each element is a constant for a simulation until solute transport equations can be coupled with the water balance, and salt sources identified and quantified. The osmotic potential of dissolved salt is approximated by the van't Hoff equation (*Metten* [1966]) by

$$\psi_s = C\,R\,T \qquad (1)$$

where C is concentration of the solution ($mol.l^{-1}$), R is the universal gas constant ($= 8.32\ l.kPa.K^{-1}.mol^{-1}$) and T is the absolute temperature (K).

An approximation here is that all salt in the root zone is dissolved in the water present; there is no check of the solution becoming saturated. Also, because there is no coupled heat dynamics equation, then on the daily timestep, we assume that the soil temperature in *(1)* is the average daily air temperature.

4.5.2.4 Relative Water Availability. Relative water availability is calculated as a function of the sum of the potentials of water and salt. The relationship used in Topog_IRM is a linear function of the sum of these potentials. The water availability is *1.0* when the sum of potentials is zero, *ie.* if no salt is present and the soil is saturated with water, and it decreases linearly to *0.0* when the sum of potentials equals or exceeds some maximum leaf water potential. Evidence for this form of relationship is presented in *Wong et. al.* [1985] for *Zea mays*.

The water availability calculation does not take into account the concept of anaerobosis, where a plant's roots may become starved of oxygen because the soil is saturated with water. This phenomenon is highly species dependent both for the point at which the effect is seen, and the magnitude of the effect.

4.5.2.4 Carbon Dioxide Concentration and Canopy Conductance. The internal leaf CO_2 concentration, in parts per million, is required in our calculation of canopy conductance; this is the reciprocal of surface resistance of the canopy. Since atmospheric concentration of CO_2 is constant for our purposes, we need only to modify this to the leaf's internal concentration. *Wong and Dunin* [1987] derived an empirical relationship between internal and external leaf CO_2 concentration for *E. maculata* Hook based on vapour pressure deficit. It is

$$[CO_2]_{leaf} = [CO_2]_{atmos}\ (0.96 - 0.0194\ vpd) \qquad (2)$$

where vpd is the vapour pressure deficit between the leaf and atmosphere.

From there, we can calculate canopy conductance according to *Ball et. al.* [1987] by

$$cc = 0.001 + g1\ A\ h\ /\ [CO_2]_{leaf} \qquad (3)$$

where $g1$ is an empirical constant for each plant species, A is todays actual assimilation, and h is relative humidity.

4.5.2.5 Surface Resistance to Evaporation. An important term with implications for other parts of the model, is the surface resistance of the soil. This calculation is taken from *Choudhury and Monteith* [1988] and is formulated as

$$r_s = \frac{\tau\, l}{p\, \mathcal{D}_v} \qquad (4)$$

where τ is tortuosity factor (constant τ=2), l is resistance length, depth of drying front, p is soil porosity, and $\mathcal{D}_v$ is the molecular diffusion coefficient for water vapour (constant $\mathcal{D}_v=2.5x10^{-5}\ m^2 s^{-1}$).

The value for l in *(4)* is taken to be the first soil depth node if the soil is not airdry, and the depth of drying front if the surface is airdry. For a minimum surface resistance of 100 say, then if the soil had $p=0.4$, the first depth node for the soil must be $0.0005\ m$. Increasing the first depth node will increase the minimum surface resistance; this can give the effect of a mulch layer.

Experience using the Richards equation for water balance modelling suggests that the depth node spacing must reflect the scale of the process being modelled. Evaporation and drying fronts are small scale processes and therefore require closely spaced depth nodes at the surface to be modelled accurately. A common rule for generating near surface depth nodes is to set your base line surface resistance, calculate your first depth node spacing, then simply double that spacing until an appropriate maximum is reached. This spacing can be continued for the rest of the layer.

5. Summary

Topog_IRM is a versatile means by which the water balance of three-dimensional catchments may be modelled, and coupled with an energy balance and plant growth. Its versatility arises from the physically (and physiologically) based approach to the modelled processes. The cost of this approach is a detailed specification of soil, climate, vegetation and topography. However, given an adequate characterisation of these data, the model should be applicable to a wide variety of research and management questions related to catchment hydrology.

A1. Appendix 1 - Derivation, Formulation and Solution of the Richards Equation in Topog_IRM

A more thorough discussion of the historical details, previous work done, and current development of the Richards equation, than presented here, is currently drafted and awaiting review.

A1-1. Water Balance Model Assumptions

As discussed in *§4.3*, the water balance module of Topog_IRM makes the following assumptions:

- that vertical movement occurs via an isothermal, isotropic, incompressible and nonhysteretic soil matrix (this assumption is explicit in using the Richards equation)
- that water movement is in the liquid phase only
- that lateral flow occurs only via a saturated watertable which is parallel to the ground surface, and those fluxes are described by Darcys' Law using the surface slope
- that macropore effects can be represented as a bulk soil property, at the spatial scale of an element, within the soil hydraulic model
- that pipes and any other large preferred pathway mechanisms do not operate
- that in one timestep, currently one day, only one sign of flux operates at the surface, *ie*. either rainfall or evaporation, and that the flux is constant over that timestep
- that any water ponded on the surface appears as outflow within the timestep.

A1-2. Definitions

The Richards Equation applies to an isothermal, isotropic, incompressible and nonhysteretic soil matrix. In this application it is applied in 1-dimension only,that is, vertical only. The units used by convention are metres (*m*) and days (*d*).

z	depth (*m*) below soil surface, that is, positive downwards
t	time (*d*)
ψ	water potential (*m*)
θ	volumetric water content (m^3/m^3)
C, θ'	differential moisture capacity, $C = \partial\theta / \partial\psi$
K	hydraulic conductivity (*m/d*)
K'	partial differential of K with respect to ψ
D	diffusivity

$$D = K\frac{\partial\psi}{\partial\theta}$$

U	Kirchhoff transform

$$U = \int_{-\infty}^{\psi} K\partial\psi \equiv \int_{0}^{\theta} D\partial\theta$$

q	moisture flux in z-direction ($m^3/d/m^2$)

Subscripts and superscripts used are as follows -

b	backward difference
f	forward difference
c	central difference
j	beginning of time step
$j+1$	end of time step
s	saturated condition, *ie.* $\psi=0$

A1-3. Basic Equations

Richards [1931] combined directly a continuity equation,

$$\frac{\partial\theta}{\partial t}=-\frac{\partial q}{\partial z} \tag{A1}$$

and Darcy's law,

$$q=K\left(1-\frac{\partial\psi}{\partial z}\right) \tag{A2}$$

to produce, in one dimension

$$\frac{\partial\theta}{\partial t}=-\frac{\partial}{\partial z}\left(K\left(1-\frac{\partial\psi}{\partial z}\right)\right) \tag{A3}$$

Equation (A3) is the fundamental mixed form of the Richards equation, and given the stated assumptions, it is applicable at any point in space or time and represents vertical moisture dynamics fully.

For analytic solutions and common numerical solution techniques, (A3) is often cast with a single dependent variable. The ψ-based form was used by Richards, and has traditionally been seen as mandatory to treat soils that may become saturated. It substitues the LHS of the equation with C, the differential moisture capacity, to produce

$$C\frac{\partial\psi}{\partial t}=-\frac{\partial}{\partial z}\left(K\left(1-\frac{\partial\psi}{\partial z}\right)\right) \tag{A4}$$

This form of the equation is highly non-linear, and has always been very hard work numerically, without having good mass balance. Good mass balance is difficult because the difference form of the C is not the same as the differential form.

The other common single dependent variable form substitutes θ into the RHS of (A3), and is commonly known as the Fokker-Planck equation. It is

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}\left(D\frac{\partial\theta}{\partial z}\right)-\frac{\partial K}{\partial\theta}\frac{\partial\theta}{\partial z} \tag{A5}$$

This form has been used for analytic solutions in the unsaturated region of a uniform soil, and has good mass balance. It follows from Richards that all forms of the equation are suitable for modelling saturated and layered soils if $\psi(\theta)$ is monotonic in the range of ψ and θ used.

A criterion for choosing a form of the equation is the need to minimise nonlinearity in time and space. *Brutsaert* [1971] presented the Richards equation as (A3) for saturated and layered soils. Redinger *et. al.* [1984] and *Ross and Bristow* [1990] minimised nonlinearity in time by using θ on the LHS, and reduced nonlinearity in space by substituting the Kirchhoff transform on the RHS. This substitution into (A3) produces

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K - \frac{\partial U}{\partial z}\right) \tag{A6}$$

Ross and Bristow found that computational effort was reduced by over two orders of magnitude, approximately a factor of 200, by the use of (A6) over the traditional (A4) with the Campbell soil model. They described how the Newton-Raphson solution scheme allowed the multiple dependent variables in (A6) to be solved, that it was applicable to saturated and layered soils, and that mass balance was reduced to computational round-off errors (order of 10^{-15}). Equation (A6) is the form chosen for solution in Topog dynamic simulations.

A1-4. The Soil-Moisture Characteristic and Monotonicity past Saturation

The Broadbridge-White soil hydraulic model has five (5) parameters only. They are K_s, θ_s and θ_r, λ_c and C. (This "C" is not to be confused with the differential moisture capacity θ' or C. All mention of "C" in this document from this point onward is a reference to the "C" used in this soil hydraulic model.)

K_s is the saturated hydraulic conductivity, as measured by an infiltrometer. It is a natural rate scaling value, thus dimensionless rate variables can be described as

$$K^* = K / K_s$$
$$q^* = q / K_s$$
$$R^* = R / K_s$$

where R is rainfall.

θ_s and θ_r are the volumetric water content of the soil at saturation and when airdry respectively. These parameters are simple to measure gravimetrically.

λ_c is a natural length scaling value, and is derived primarily from sorptivity. Dimensionless length variables can be described as

$$z^* = z / \lambda_c$$
$$\psi^* = \psi / \lambda_c$$

C is a shape parameter related to soil structure, and has a range of $1 < C < \infty$, although it has a practical range in nature from about 1.02 to 1.5. Its value may be estimated from a simple infiltration experiment.

A third natural scale that emerges from the Broadbridge-White soil model is called t_c. It scales time and is formulated as

$$t_c = \frac{\lambda_c \Delta \theta}{K_s}$$

and thus dimensionless time can be described as

$$t^* = t / t_c$$

The soil hydraulic functions are derived starting from diffusivity, and ensuring that it neither tends toward zero as $\psi \to -\infty$, nor tends toward ∞ as $\psi \to 0$. Broadbridge and White defined the soil hydraulic functions, shown here in dimensional and dimensionless forms, as

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

$$\psi \frac{1}{\lambda_c} = \psi^* = \frac{\Theta - 1}{\Theta} - \frac{1}{C} ln\left(\frac{C - \Theta}{\Theta(C-1)}\right)$$

$$K \frac{1}{K_s} = K^* = \frac{\Theta^2 (C-1)}{C - \Theta}$$

$$U \frac{1}{K_s \lambda_c} = U^* = \frac{K^*}{\Theta}$$

$$\frac{\partial \theta}{\partial \psi} \frac{\lambda_c}{\Delta \theta} = \frac{\partial \Theta}{\partial \psi^*} = \frac{\Theta^2 (C - \Theta)}{C}$$

$$\frac{\partial K}{\partial \psi} \frac{\lambda_c}{K_s} = \frac{\partial K^*}{\partial \psi^*} = \frac{\Theta^3 (C-1)(2C - \Theta)}{C(C - \Theta)}$$

As mentioned before, any form of the Richards equation can be used so long as the dependent variables are single valued functions throughout the entire range of application. Since we want to apply this scheme up to and past the point of saturation, *ie*. when $\psi \geq 0$, then the relation between ψ and θ must be monotonic always. This condition flows naturally from the Broadbridge-White soil model, since it holds over the entire unsaturated range, and $\partial\theta / \partial\psi = \Delta\, \theta (C-1) / (C \lambda_c) > 0$ at $\psi = 0$. The $\psi(\theta)$ function is extended beyond saturation by reducing the dimensionless derivative value at $\psi^* = 0$ exponentially, until a suitably small value is reached, afterwhich it remains constant, and then calculating θ based on the derivative. For our purposes, a dimensionless value of 10^{-4} was chosen. It will increase the value of θ by 1% of θ_s for every +100m of water pressure past the terminal point. A similar method and cutoff is used for continuing the $\psi(K)$ curve, and the calculation of K and U past saturation.

A1-5. Guaranteed Convergence using Broadbridge-White Soil Model

It is desirable that the user have some idea that they will not wait for an hour of CPU time only for the Richards equation code to fail to converge just as the action begins. The Broadbridge-White soil model possesses another level of linear dimensionless scaling, that removes the soil factor from the variables. In short you are left with a rainfall rate on a general soil. Given that we have a fixed timestep, then we need to run simulations changing only the rainfall rate and depth node spacing to find the space in which we can guarantee convergence. For the actual numerical exercise, different levels of timestep were imposed, but had no effect on the final result.

The second level of scaling defines the following functions

$$m = 4C(C-1)$$

$$\Theta^{\#} = \Theta/C$$

$$\psi^{\#} = C\psi^{*}$$

$$K^{\#} = K^{*}/m$$

$$D^{\#} = D^{*}C^{2}/m$$

$$U^{\#} = U^{*}C/m$$

$$z^{\#} = C\,z^{*}$$

$$\tau = m\,t^{*} \qquad \text{(dimensionless time)}$$

$$\rho = R^{*}/m \qquad \text{(dimensionless rainfall)}$$

With a new soil hydraulic model defined as above, the user need only specify ρ, $\Delta\tau$ and $\Delta z^{\#}$, and the simulation will be applicable to every combination of raw dimensional input parameters.

The result of many simulations can be boiled down into a single rule of thumb - ***for almost all real rainfall rates on soils with realistic* C *values, if the depth node spacing is kept to* λ_c *or below, convergence is guaranteed***. Further, given the maximum rate that water can flow into a lower layer is K_s, which is a realistic rainfall rate, then ***the same rule applies to every layer*** and infact ***to the whole layered system***.

The program that generates Broadbridge-White soil table has the capability of producing a table of functions of other popular soil models. If natural scaling occured in these other soil models as occurs in Broadbridge-White, then a rule of thumb could be generated for each. To the present time, such features have not been shown or used, so no guarantees of convergence can be given for any other soil models.

A1-6. Newton-Raphson Solution Scheme

Equation (A1) can be represented in finite difference form at a depth node i, over time j to $j+1$, with a variable temporal weighting, and central difference in space as

$$F_i = \alpha\left(q_{i+0.5}^{j+1} - q_{i-0.5}^{j+1}\right) + (1-\alpha)\left(q_{i+0.5}^{j} - q_{i-0.5}^{j}\right) + e_i = 0 \tag{A7}$$

where

$$e_i = \left(\theta_i^{j+1} - \theta_i^{j}\right)\frac{\Delta z_{ci}}{\Delta t_{fi}} \tag{A8}$$

and

$$q_{i+0.5}^{j} = K_{i+0.5}^{j} - \frac{U_{i+1}^{j} - U_i^{j}}{\Delta z_{fi}} \tag{A9}$$

$$K_{i+0.5}^{j} = \sqrt{K_i^j K_{i+1}^j} \tag{A10}$$

Equation (A7) is modified at the upper, node 0, and lower, node n, boundaries, to give

$$F_0 = \alpha\left(q_{0.5}^{j+1} - q_0^{j+1}\right) + (1-\alpha)\left(q_{0.5}^{j} - q_0^{j}\right) + e_0 = 0 \tag{A11}$$

$$e_0 = \left(\theta_0^{j+1} - \theta_0^{j}\right)\frac{\Delta z_{f0}}{2\Delta t_{fi}} \tag{A12}$$

and

$$F_n = \alpha\left(q_n^{j+1} - q_{n-0.5}^{j+1}\right) + (1-\alpha)\left(q_n^{j} - q_{n-0.5}^{j}\right) + e_n = 0 \tag{A13}$$

$$e_n = \left(\theta_n^{j+1} - \theta_n^{j}\right)\frac{\Delta z_{fn-1}}{2\Delta t_{fi}} \tag{A14}$$

In (A11), q_0 is taken as rainfall or evaporation rate, and in (A13), q_n is taken to be recharge or discharge, or a term to describe lateral fluxes.

The value of the temporal weighting α is interesting:

- $\alpha=1.0$ indicates a backward difference, or fully implicit formulation that uses little information from the previous timestep
- $\alpha=0.5$ indicates a Crank-Nicolson formulation which uses fluxes and other values from the previous timestep
- $\alpha=0.0$ is a forward difference, or fully explicit formulation; this scheme has tight restrictions on the allowable Δz and Δt.

We use $\alpha=1.0$ for minimising the amount of storage required, number of arithmetic operations, and because of its slightly larger area of guaranteed convergence over $\alpha=0.5$.

The Newton-Raphson solution scheme solves a matrix equation of the form

$$-[F] = [\partial F/\partial \psi^{j+1}][\Delta \psi] \quad \text{(A15)}$$

where $[F]$ is based on the current estimate of $[\psi]$, and the solution vector is a correction to $[\psi]$ which is applied by

$$[\psi_{new}] = [\psi_{old}] - [\Delta \psi] \quad \text{(A16)}$$

and our new estimate of $[\psi]$ will update $[F]$. Thus (A15) is solved iteratively, until each F_i, equation (A7), satisfies a suitably small tolerance. In our case, we use a criteria that all $|F_i| < 10^{-10}$.

To generate the matrix $[\partial F/\partial \psi^{j+1}]$, we take the derivative of each F_i with respect to the solution variable. Because we want this to apply to both saturated and layered soils, we have selected ψ since it is continuous through saturation and across soil boundaries. Each F_i has three derivatives at $j+1$, one each with respect to ψ at $i-1$, i and $i+1$. The exceptions are the surface and lower boundary nodes; these have only two derivatives. The resulting Jacobian matrix is tridiagonal, and the solution of (A15) is subject to very efficient techniques. The three derivatives at $j+1$ for each internal node i are as follows

$$\frac{\partial F_i}{\partial \psi_{i-1}} = -\frac{K'_{i-1}}{2}\sqrt{\frac{K_i}{K_{i-1}}} - \frac{K_{i-1}}{\Delta z_{fi-1}} \quad \text{(A17)}$$

$$\frac{\partial F_i}{\partial \psi_i} = \frac{K'_i}{2}\left(\sqrt{\frac{K_{i+1}}{K_i}} - \sqrt{\frac{K_{i-1}}{K_i}}\right) + K_i\left(\frac{1}{\Delta z_{fi-1}} - \frac{1}{\Delta z_{fi}}\right) + \frac{\theta_i \Delta z_{ci}}{\Delta t_{fj}} \quad \text{(A18)}$$

$$\frac{\partial F_i}{\partial \psi_{i+1}} = \frac{K'_{i+1}}{2}\sqrt{\frac{K_i}{K_{i+1}}} - \frac{K_{i+1}}{\Delta z_{fi}} \quad \text{(A19)}$$

At node 0 there is no derivative with respect to ψ_{i-1}, and at node n there is no derivative with respect to ψ_{i+1}. The two derivatives for node 0 are

$$\frac{\partial F_0}{\partial \psi_0} = \frac{K'_0}{2}\sqrt{\frac{K_1}{K_0}} + \frac{K_0}{\Delta z_{f0}} + \frac{\theta_0 \Delta z_{f0}}{2\Delta t_{fj}} \quad \text{(A20)}$$

$$\frac{\partial F_0}{\partial \psi_1} = \frac{K'_1}{2}\sqrt{\frac{K_0}{K_1}} - \frac{K_1}{\Delta z_{f0}} \quad \text{(A21)}$$

and the two derivatives for node n are

$$\frac{\partial F_n}{\partial \psi_{n-1}} = -\frac{K'_{n-1}}{2}\sqrt{\frac{K_n}{K_{n-1}}} - \frac{K_{n-1}}{\Delta z_{fn-1}} \quad \text{(A22)}$$

$$\frac{\partial F_n}{\partial \psi_n} = -\frac{K'_n}{2}\sqrt{\frac{K_{n-1}}{K_n}} + \frac{K_n}{\Delta z_{fn-1}} + \frac{\theta_n \Delta z_{fn-1}}{2\Delta t_{fj}} \quad \text{(A23)}$$

All extra fluxes for node i, are added into (A13), and if they have a derivative with respect to ψ, then that derivative is added to (A18). For example, we have a lateral flow component in Topog that is a function of the watertable depth. $\psi > 0$ at node n indicates a saturated watertable, and the ψ value is the depth. The flux of water leaving the element is calculated according to Darcys Law by

$$q_c = \psi_n K_s m w / A \qquad \text{(A24)}$$

where m is slope, w is width of the element, and A is the area of the element. The derivative of q_c with respect to ψ_n is

$$\frac{\partial q_c}{\partial \psi_n} = K_s m w / A \qquad \text{(A25)}$$

The result of (A24) is "added" to (A13) (subtracted in this case to account for sign), and the result of (A25) is "added" to (A23). The fluxes are divided by the area of the element A, to reduce them to a unit area basis. This representation of lateral flux is backward difference, since it assumes that the saturated watertable is parallel to the surface gradient, *ie*. the depth of the watertable is constant over the entire element.

Fluxes that are introduced at each depth node are plant transpiration fluxes. In Topog_IRM these fluxes are calculated for conditions at the beginning of the time step, and are applied as constant for the whole time step. Each depth node is assigned a flux that is "subtracted" from the water balance of the node in (A7), but nothing is "subtracted" from (A13) because the derivative with respect to ψ is zero for all nodes.

The equations so far are representative of a flux boundary condition at the surface. The other possible boundary condition at the surface is one of fixed potential. This condition occurs when water ponds on the soil surface, or when there is so much evaporative demand that the surface becomes airdry. Under either of these conditions, a triangle of mass representing the difference between the current surface potential and that which we will impose is first determined, then the iterative solution is run, but starting at node *1* using internal and lower boundary equations only, but omitting (A17). We can ignore (A17) at node *1* because ψ_0 can not change, since it is a constant potential, and therefore any derivative with respect to it will be zero.

Along with the convergence criteria expressed earlier, we must also restrict the change in ψ_i between iterations. This is because using a tangent method such as Newton-Raphson, small derivatives can indicate very large changes between estimates. The criterion used by Ross and Bristow was

$-\Delta\psi_i < -0.8\psi_i$, for $\psi_i < -0.1m$ and $\Delta\psi_i < 0$

no restriction otherwise

This is effectively a uni-directional criterion that restricts the rate at which the soil can become wetter when unsaturated. One problem it can create is that at one node $\psi \to -\infty$, and the solution cannot get back on track. This would be unacceptable in a general model where hundreds or thousands of soil columns are being solved for each timestep. The factor of *0.8* is somewhat arbitrary, but prevents a node from reaching saturation in a single iteration; a limited investigation found this to be important.

The criterion used in the Topog_IRM solution is

$|\Delta\psi_i| < 0.8|\psi_i| + k$, for $\psi_i < 0$

where k is the positive ψ value at which the derivatives of θ and K reach their constant value. This condition prevents both rapid wetting and drying from occurring, while providing restriction over a greater range than Ross and Bristow. There is no restriction in the saturated range because ψ changes slowest here, and the derivatives are nearly constant providing an almost linear solution.

A1-7. Formulation for Layered or Gradational Soil

Consider equations (A7) and (A8) above and below a soil interface. Using $\alpha=1.0$, the subscript u for upper layer, and l for lower layer, we can write

$$F_u = q_{u,i}^{j+1} - q_{u,i-0.5}^{j+1} + e_{u,i} = 0 \qquad \text{(A25)}$$

where

$$e_{u,i} = \left(\theta_{u,i}^{j+1} - \theta_{u,i}^{j}\right)\frac{\Delta z_{bi}}{2\Delta t_{fj}} \qquad \text{(A26)}$$

and

$$F_{l,i} = q_{l,i+0.5}^{j+1} - q_{l,i}^{j+1} + e_{l,i} = 0 \qquad \text{(A27)}$$

where

$$e_{l,i} = \left(\theta_{l,i}^{j+1} - \theta_{l,i}^{j}\right)\frac{\Delta z_{fi}}{2\Delta t_{fj}} \qquad \text{(A28)}$$

By recognising that ψ and q are continuous across a layer boundary, then by adding (A25) to (A27) we get

$$F_i = q_{l,i+0.5}^{j+1} - q_{u,i-0.5}^{j+1} + e_{u+l,i} \qquad \text{(A29)}$$

where

$$e_{u+l,i} = \frac{1}{2\Delta t_{fj}}\left(\left(\theta_{u,i}^{j+1} - \theta_{u,i}^{j}\right)\Delta z_{bi} + \left(\theta_{l,i}^{j+1} - \theta_{l,i}^{j}\right)\Delta z_{fi}\right) \qquad \text{(A30)}$$

The derivatives of (A29) and (A30) will now contain a mixture of derivatives and variables, the derivative or value with respect to the layer you are within. Superficially though, only the e_i really changes at a soil boundary.

An additional convergence restriction is required in layered soils, due to the nature of their solution. The corrections of [ψ] tend to oscillate in sign over a very small range about the correct solution. To remove the effect of these oscillations, ***if the correction to any ψ_i changes sign between iterations, then the magnitude of the change is halved***. This means that if the corrector was oscillating in sign only, then by halving the magnitude we must fall on the correct solution. This criteria is applied regardless of whether layers are present without penalty.

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