



# Fast Solution of Richards' Equation for Flexible Soil Hydraulic Property Descriptions

Peter J. Ross

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# 1. Executive Summary

Fast methods of solving the Richards equation for soil water transport and the advection-dispersion equation for solute transport are important in areas where large numbers of solutions are required. This report extends the work of Ross (2003) on fast methods of solution to more general soil hydraulic properties. The solution depends on the combination of several methods. First, use of the matric flux potential (Kirchhoff transform) for calculating water fluxes allows relatively large nodal spacing in the spatial discretisation. Second, appropriate weighting of nodal hydraulic conductivities in calculating water fluxes due to gravity ensures a stable and acceptably accurate solution. Third, use of a non-iterative time-stepping method that allows the time step to be adjusted for various conditions ensures a fast, accurate, robust solution. Conditions monitored include changes in nodal water contents, which are used as an overall control of step size, saturation and desaturation at nodes, formation and disappearance of surface ponds and runoff at a specified pond depth. Fourth, use of water content as the dependent variable in unsaturated regions ensures accurate mass balance. Fifth, using a time weighting of 0.5 for water fluxes when the profile is unsaturated and a fully implicit weighting of 1 only when there are saturated nodes improves accuracy without compromising stability. Finally, the advection-dispersion equation for multiple non-interacting solutes is solved only after a preset number of time steps using averaged water fluxes. This allows treatment of nonlinear adsorption isotherms without unduly increasing the overall solution time.

The previous work used Brooks and Corey (1964) soil hydraulic properties. Here the more general water retention function of van Genuchten (1980) is used. This function is modified to remove the slope singularity at saturation by making the head  $h$  a quadratic function of effective saturation  $S$  for  $S > S_1$ , where  $S_1$  is close to 1 ( $\approx 0.99$ ). In dry soil a logarithmic water retention function may optionally be used. Two hydraulic conductivity formulations are considered. The first is that of Brooks and Corey (1964), optionally combined with "macropore" components that decrease exponentially with suction. The second is that of Schaap and van Genuchten (2005), which is implemented using quadratic approximation of the  $K(h)$  function at lower suctions.

The only boundary conditions previously considered were ponding at the surface and free drainage (unit hydraulic gradient) at the base. Now added are a preset pond depth at the surface and constant head, seepage and zero flux at the base.

Several Fortran 90 computer routines have been written for illustration and application of the methods. Included in them is a simple model of water extraction by plants taken from the literature.

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## 2. Introduction

In recent years faster computers and more efficient computing methods have extended areas of application of numerical solutions of the Richards equation (RE) for soil water transport and the advection-dispersion equation (ADE) for solute transport. However, areas such as large-scale hydrological models, stochastic models, uncertainty estimation and two or three dimensional models can still benefit from faster solutions. Ross (2003) described new, faster methods for both the RE and the ADE. Solution of the RE was accomplished using a robust non-iterative method that took special account of saturating and desaturating soil layers while the cost of simultaneously solving the ADE was minimised by averaging the water fluxes over several time steps. The RE solution was based on the Brooks and Corey (1964) (BC) formulation of soil hydraulic properties and was thus of limited applicability. This report extends the methodology to more general forms of soil hydraulic properties. The water retention function of van Genuchten (1980) (vG) is modified near saturation to remove the slope singularity and make it more friendly numerically. An optional logarithmic function is joined to it to better describe retention in dry soil. Optional exponential components are joined to the BC conductivity function to better describe “macropore” conductivity in wet soil. Alternatively, the conductivity model of Schaap and van Genuchten (2005) (SvG) may be used. Several Fortran 90 computer routines have been written for illustration and application. The reader is assumed to be familiar with the material in Ross (2003), which will not be repeated here.

## 3. Hydraulic Properties

### 3.1. Hydraulic Properties near Saturation

The RE solution uses the degree of saturation

$$S = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (1)$$

as the state variable in unsaturated regions, where  $\theta$  is the water content ( $\text{cm}^3 \text{cm}^{-3}$ ),  $\theta_r$  is the residual water content and  $\theta_s$  the saturated water content. The matric flux potential (MFP)  $\phi$  ( $\text{cm}^2 \text{h}^{-1}$ ) is the state variable in saturated regions, where it is linearly related to the matric head  $h$  (cm), which is taken as negative in unsaturated soil. It is also used to calculate water fluxes in both saturated and unsaturated regions. As well as a dimensionless water content, a dimensionless relative head  $h_r$  can be defined in terms of a head scaling parameter. For the BC water retention function, saturation occurs at an “air entry” head  $h = h_e$  that can be used as the scaling parameter. Then

$$S(h) = h_r^{-\lambda}, \quad h_r = h / h_e \quad (2)$$

where  $\lambda$  is a shape parameter. For the vG retention function,

$$S(h) = (1 + h_r^n)^{-m}, \quad h_r = \alpha |h| = h / h_g \quad (3)$$

where  $h_g = -1/\alpha$  is the head scaling parameter (Fuentes *et al.* 1992) and the shape parameters  $m$  and  $n$  are related by

$$m = 1 - k_{vG} / n, \quad (4)$$

with  $k_{vG}$  usually taken to be 1 or 2.

With many functions in use, including the vG function, saturation occurs at  $h = 0$  and the slope of the curve close to saturation can cause problems in some numerical solutions if allowance for it is not made. In addition, the vG hydraulic conductivity function decreases too sharply near saturation in most field soils. It has therefore been found convenient to modify the water retention curve slightly so that saturation occurs at a non-zero head, which may be only one or two centimetres (Vogel and Cislárová 1988; Vogel *et al.* 2001; Schaap and van Genuchten 2005). Here a different approach is taken so that saturation still occurs at  $h = 0$ , allowing “macropore” components of the conductivity to be added in the unsaturated region. For  $S > S_1$ , where  $S_1$  is close to 1 (e.g. 0.99),  $h$  is defined as a quadratic function of  $S$  with the same value and slope at  $S_1$  as the van Genuchten function and a value of 0 at  $S = 1$ . This removes the infinite slope at  $S = 1$  that is present in the vG  $h(S)$  function and results in a curve that is effectively indistinguishable from it experimentally. The water retention function is then defined by

$$\begin{aligned} h_r(S) &= (S^{-1/m} - 1)^{1/n}, & S \leq S_1 \\ &= a_1 \left( \frac{S-1}{S_1-1} \right) + a_2 \left( \frac{S-1}{S_1-1} \right)^2, & S > S_1 \end{aligned} \quad (5)$$

where

$$a_1 = 2h_{r1} - (S_1 - 1)(dh_r/dS)_1, \quad a_2 = h_{r1} - a_1. \quad (6)$$

Here  $h_{r1}$ ,  $(dh_r/dS)_1$  are the value and slope of the vG function at  $S_1$ . The inverse function is

$$\begin{aligned} S(h_r) &= (1 + h_r^n)^{-m}, & h_r \geq h_{r1} \\ &= 1 + 2(S_1 - 1)h_r / \left( a_1 + \sqrt{a_1^2 + 4a_2 h_r} \right), & h_r < h_{r1} \end{aligned} \quad (7)$$

The BC hydraulic conductivity function for the “soil matrix” is, for the BC retention function,

$$K(h_r) = K_x h_r^{-\lambda \eta} \quad (8)$$

and for the vG retention function

$$K(h_r) = K_x (1 + h_r^n)^{-m \eta}. \quad (9)$$

where  $K_x$  is the saturated conductivity of the “soil matrix” ( $\text{cm h}^{-1}$ ) and  $\eta$  is a parameter usually related to the retention curve parameters  $\lambda$ , or  $m$  and  $n$ , e.g. by the relations used here (Campbell 1985, Fuentes *et al.* 1992)

$$\eta = \frac{2}{\lambda} + 2 + p \quad \text{or} \quad \eta = \frac{2}{mn} + 2 + p \quad (10)$$

where  $p$  is a “pore interaction parameter” in the conductivity model used. These relations imply a correspondence between  $\lambda$  and  $mn$ . On the basis of the shape of the retention curve, Haverkamp *et al.* (2005) and Leij *et al.* (2005) have suggested another where, for  $\theta_r = 0$ ,  $\lambda$  corresponds to  $mn / (1 + m)$ . In practice, any relation can be accommodated by an appropriate choice of  $p$ .

Soil structural features, usually termed “soil macroporosity”, frequently increase the hydraulic conductivity near saturation well above that of the “soil matrix”. The porosity due to these features may be small and as a simplification can be ignored or assumed to be included in

the retention function. A “macropore” conductivity that decreases exponentially with  $h$  from saturation is given by

$$K_{mp}(h) = K_p \exp[-h/h_p], \quad (11)$$

where  $K_p$  is the value at saturation and  $h_p$  determines the rate of decrease. This conductivity function is used when  $h$  is greater than some assigned head  $h_{mac}$ , provided  $h_{mac} < 0$ . The parameter  $h_p$  is calculated from  $K_p$  and the value of  $K$  at  $h_{mac}$ . In case an extra increase in  $K$  is required close to saturation, a second similar function joining the first can be used there.

The SvG conductivity function is

$$K(h) = \left( \frac{K_s}{K_{vGm}(h)} \right)^{R(h)} K_{vGm}(h) \quad (12)$$

where

$$\begin{aligned} R(h) &= 1 - (1 - R_{mac1})h/h_{mac1}, & 0 \geq h \geq h_{mac1} \\ &= \frac{R_{mac1}(h - h_{mac2})}{h_{mac1} - h_{mac2}}, & h_{mac1} > h \geq h_{mac2} \\ &= 0, & h < h_{mac2} \end{aligned} \quad (13)$$

and  $K_{vGm}(h)$  is a modified version of the vG conductivity function

$$K(h) = K_x x^{mp} (1 - (1 - x)^m)^2 \quad (14)$$

given by

$$\begin{aligned} K_{vGm}(h) &= K_x \frac{x^{mp} (1 - (1 - x)^m)^2}{x_s^{mp} (1 - (1 - x_s)^m)^2} = K_{xm} x^{mp} (1 - (1 - x)^m)^2, & h < h_s \\ &= K_x, & h \geq h_s \end{aligned} \quad (15)$$

with  $x = 1/(1+h_r^n)$  and  $x_s$  the value of  $x$  at the “soil matrix” saturation head  $h_s$  which is a small negative head taken equal to  $h_{mac1}$ . Suggested values are  $h_{mac1} = -4$  cm,  $h_{mac2} = -40$  cm and  $R_{mac1} = 0.25$ . Note that  $K = K_{vGm}$  for  $h < h_{mac2}$ . Note also that  $K$  is an exponential function of  $h$  for  $h \geq h_{mac1}$ .

### 3.2. Hydraulic Properties near Dryness

The value of the head  $h$  at oven dryness, when the water content is by definition zero, is approximately  $-10^7$  cm (Ross *et al.* 1991). The retention curve from  $h = -10^7$  cm to  $h = -10^5$  cm or higher (up to  $-15000$  cm) is often described by a logarithmic function of  $h$  (McQueen and Miller 1974; Campbell and Shiozawa 1992; Rossi and Nimmo 1994) which may simply join the curve used for larger values of  $h$  at a point  $(h_j, S_j)$ . Thus,

$$S(h) = \left( \frac{S_j}{\ln(h_j/h_d)} \right) \ln(h/h_d), \quad h_d \leq h < h_j \quad (16)$$

where  $h_d = -10^7$  cm and residual water content  $\theta_r = 0$ . Applying the generalised conductivity model discussed by Hoffmann-Riem *et al.* (1999) gives

$$K_{\log}(h) = K_j \left( \frac{S(h)}{S_j} \right)^a \left( \frac{h^{-b} - h_d^{-b}}{h_j^{-b} - h_d^{-b}} \right)^c, \quad (17)$$

where  $K_j$  is the conductivity at the join. Because there is a paucity of measurements, the error in applying a model based on capillarity to a region where forces are adsorptive is not known. The values of  $a$ ,  $b$  and  $c$  may be chosen for convenience from among those commonly used, in particular  $a = 0$ ,  $b = 2$  and  $c = 1$ . Allowing  $b$  to vary adds some flexibility.

### 3.3. Matric Flux Potential

Defining the matric flux potential (MFP)  $\phi$  (Gardner 1958; Campbell 1985) as

$$\phi(h) = \int^h K(\bar{h}) d\bar{h}, \quad (18)$$

the conductivity functions above give the following.

The BC relation, Eq. (8), gives

$$\phi(h) = \frac{-h_e K_x}{\lambda \eta - 1} \left( \frac{h}{h_e} \right)^{1-\lambda \eta}. \quad (19)$$

The vG retention with the BC conductivity, Eq. (9), gives

$$\phi(h) = \frac{-h_g K_x}{n} B_x(m\eta - 1/n, 1/n). \quad (20)$$

Here B is the incomplete beta function and  $x = 1/(1+h_r^n)$  as before.

For the “macropore” component of Eq. (11),  $\phi_{mp}(h) = -h_p K_{mp}(h)$ . Neither the vG conductivity function nor the SvG modification yields a simple analytical expression for  $\phi$  and approximations must be used. The logarithmic function, Eq. (17), gives expressions involving incomplete gamma functions for integer values of  $c$ , but for the case  $a = 0$  and  $c = 1$  used here the simple result is

$$\phi_{\log}(h) = \frac{K_j}{h_j^{-b} - h_d^{-b}} \left( \frac{h^{1-b}}{1-b} - h h_d^{-b} \right). \quad (21)$$

The MFP is also called the Kirchhoff potential or transform. It is defined here as an indefinite integral, i.e., only to within an additive constant. In practice, only differences in the MFP are used, so the additive constant is irrelevant provided it is not so large as to result in significant errors in the differences.

### 3.4. Approximation of Functions

The incomplete beta function in Eq. (20) is approximated using four steps of the standard continued fraction approximation (Press *et al.* 1992). The SvG conductivity function, Eq. (12),

and  $\phi$ , its integral with respect to  $h$ , are approximated using series expansion and conversion to Padé approximations for  $h \leq h_g$  (or for  $h \leq h_{mac2}$  if  $h_{mac2} < h_g$ ). We have

$$1 - (1-x)^m \cong \frac{mx(2-x)}{2 + (m-2)x[1 + (m-1)x/6]}, \quad x \leq 1/2 \quad (22)$$

which avoids an extra exponentiation and the errors for very small  $x$  that result from subtraction during direct evaluation. The Padé approximation for  $\phi$  is

$$\phi(h) \cong h_g K_{xm} m^2 (m-1) x^a \frac{\frac{1}{a} + \left(\frac{1}{a+1} + \frac{c}{a}\right)x + \left(\frac{c}{a+1} + \frac{b}{12}\right)x^2}{1+cx}, \quad x \leq 1/2 \quad (23)$$

where

$$a = m(p+1)+1, \quad b = \frac{m^2+11}{a+2}, \quad c = \frac{-2(m^2+5)}{b(a+3)} \quad (24)$$

For  $h > h_g$  (or  $h > h_{mac2}$  if  $h_{mac2} < h_g$ ) the region from  $h_{mac1}$  to  $h_{mac2}$  is divided into  $3 + (h_{mac2} - h_{mac1}) / h_g$  segments and  $K$  is approximated in each segment by as many evenly spaced quadratics in  $h$  as are needed to achieve a specified relative error. Only the number and the defining values of  $K$  need be stored since the corresponding values of  $h$  can be calculated. The two levels of even spacing in  $h$  simplifies interpolation. A similar scheme with  $1 + (h_g - h_{mac2}) / h_g$  segments is used for the range  $h_{mac2}$  to  $h_g$  if  $x$  at  $h_{mac2}$  is greater than 0.55. If  $x$  at  $h_{mac2}$  lies between 0.5 and 0.55 the approximations above are used. Values of  $\phi$  are found by integration of the quadratics and values at the ends of each quadratic are stored. For the property types used here, and a relative error of 0.01, approximately 13 values of  $K$  and 6 of  $\phi$  were needed on average for each property type.

## 4. Computer Programs

### 4.1. Fortran Routines

The computer routines, available from the author (email address [peter.ross@csiro.au](mailto:peter.ross@csiro.au)), are written in Fortran 90, whose modules allow separation of the flow code from the hydraulic property code. There is also a (very small) module called “numbers”, which defines a Fortran real kind named RK to set the precision of real variables. On a PC there is little difference in execution speed between four and eight byte reals, but of course a large difference in memory usage. There is also a module “roots” for including uptake of water by plants, which implements the simple uptake model of Li *et al.* (2001). There is one flow module, “flow”, and three hydraulic property modules, “hypbc”, “hypvgbc” and “hypvgvg”. Module “hypbc” provides BC hydraulic properties, as in Ross (2003), but nothing else. It illustrates the essentials of a property module. Module “hypvgbc” provides vG water retention curves with BC conductivity, and includes optional “macroporosity” conductivity components and an optional logarithmic retention function in dry soil. Module “hypvgvg” provides vG retention and SvG conductivity with an optional logarithmic retention function in dry soil. Note that module “flow” contains a USE statement which must be set for whatever property module is required. Confusing error messages arise with the wrong USE statement, so it is best to use different directories for the three property modules with a copy of “flow” with the appropriate

USE statement in each. Each property module has an associated module to check the values generated (modules “chkbc”, “chkvgbc” and “chkvgvg”).

As well as the modules, there are several main programs illustrating their use. Program “ross03” reproduces results from Ross (2003) using “hypbc”. Program “isobc”, a modification of this, illustrates the use of isotherms. Apart from these, solute is not considered.

Program “hb62vgbc” reproduces results for a layered soil from Hanks and Bowers (1962) using “hypvgbc” with fitted hydraulic properties and ponded infiltration. Program “simple” uses simple but inefficient integration techniques together with a log transform of  $h$  to solve the same problem. This provides an independent check on the results. The transform, defined by

$$\begin{aligned} u &= h, & h &\geq h_0 \\ &= h_0 \ln(eh/h_0), & h &< h_0 \end{aligned} \tag{25}$$

improves accuracy and stability of the solution in dryer soil ( $h_0 \sim -50$  cm). Note that value and slope are continuous at  $h_0$ . A somewhat similar inverse sinh transform was employed by Ross (1993).

Programs “tstbc”, “tstvgbc” and “tstvgvg” solve a problem similar to that of Ross (2003), but with three 250 mm rainfall events over 1200 h, for 729 hydraulic property combinations. These programs test the speed and robustness of the code. They also use the check modules to assess errors in generated property values. Program “rexvgbc” illustrates the use of module “roots”. Program “macvgvg” uses greater “macroporosity” conductivity than “tstvgvg” while “macvgbc” produces almost the same results with BC conductivity and “macropore” components by adjusting parameters to approximate the SVG conductivities.

## 4.2. Use of the Flow Module

Several public entities are accessible in the flow module. There are also private parameters documented in the code that will not be considered here. Definitions of the public entities are as follows. More detailed information is available in the code. Units are centimetres and hours. Units for solute are arbitrary and are chosen by the user.

**botbc:** bottom boundary condition for water. This can be "constant head", "free drainage" (the default), "seepage" or "zero flux".

**h0max:** maximum pond depth before runoff occurs ( $10^{10}$  by default).

**qprecmax:** maximum precipitation (or water input) rate for use with ponded constant head infiltration ( $10^{10}$  by default). If  $qprec > qprecmax$  then actual input rate is taken to be equal to infiltration plus evaporation rates.

**hbot:** matric head at the bottom of the profile when botbc set to "constant head" (0 by default).

**dSmax:** maximum change in  $S$  of any unsaturated layer to aim for each time step. This value controls the time step size (0.05 by default).

**dSmaxr:** maximum negative relative change in  $S$  of any unsaturated layer each time step. This parameter helps avoid very small or negative  $S$  (0.5 by default).

**dtmax:** maximum time step allowed ( $10^{10}$  by default).

**dsmmax:** maximum solute change to aim for per time step of the ADE solution (1 by default).

**nwsteps:** the solute routine is called every nwsteps of the RE solution (10 by default).

**solve:** subroutine to solve the RE and the ADE.

**isosub:** subroutine to get adsorbed solute from the concentration in the soil water.

The arguments for the call to subroutine “solve” are as follows (in denotes input, out denotes output, in/out denotes both).

*Required arguments:*

**ts:** start time (in).

**tfin:** finish time (in).

**qprec:** precipitation rate or water input rate (in).

**qevap:** potential evaporation rate from the soil surface (in).

**n:** integer number of soil layers (in).

**nsol:** integer number of solutes (in).

**dx(1:n):** layer thicknesses (in).

**jt(1:n):** integer array of layer soil type numbers (in).

**h0:** surface head, equal to depth of surface pond (in/out).

**S(1:n):** degree of saturation of layers (in/out).

**evap:** cumulative evaporation from soil surface (in/out).

**runoff:** cumulative runoff (in/out).

**infil:** cumulative net “infiltration” (integral of net flux across surface) (in/out).

**drn:** cumulative net “drainage” (integral of net flux across base) (in/out).

**nsteps:** cumulative integer number of time steps for the RE solution (in/out).

*Optional arguments:*

**heads(1:n):** matric heads  $h$  of layers at finish (out). This is optional because extra function evaluations are required.

**qexsub:** subroutine to get layer water extraction rates ( $\text{cm h}^{-1}$ ) by plants. There is no solute extraction and osmotic effects due to solute are ignored; nor is there extraction from saturated layers.

**wex(1:n):** cumulative water extraction from layers (in/out).

**cin(1:nsol):** solute concentrations in water input (user's units per  $\text{cm}^3$ ) (in).

**c0(1:nsol):** solute concentrations in surface pond (in/out).

**sm(1:n,1:nsol):** solute concentrations in layers (in/out).

**soff(1:nsol):** cumulative solute runoff (in/out).

**sinfil(1:nsol):** cumulative solute infiltration (in/out).

**sdrn(1:nsol):** cumulative solute drainage (in/out).

**nssteps(1:nsol):** cumulative integer number of time steps for the ADE solution (in/out).

**isosub:** subroutine to get adsorbed solute from concentration in the soil water.

Arguments for subroutine “qexsub” (see module “roots” for an example) are as follows.

**jt(1:n):** layer soil type numbers (in).

**h(1:n):** layer matric heads (in).

**qex(1:n):** layer extraction rates (out).

**qexh(1:n):** partial derivatives of  $qex$  with respect to  $h$  (out).

There is a usable example of subroutine “isosub” with the same name provided in the flow module. Arguments for “isosub” are as follows.

**iso:** 2 character code (in). In the routine provided, “Fr”, “La” and “LI” designate Freundlich, Langmuir and Langmuir-linear. A code “li” for linear is built into the flow module and requires no subroutine.

**c:** concentration in soil water (in).

**p(:):** isotherm parameters (in/out).

**f:** adsorbed mass per gram of soil solids (out).

**fc:**  $df/dc$ ; i.e., slope of the isotherm curve (out).

The flux calculations at soil type interfaces in Ross (2003) stored and updated  $\phi$  above the interface. Here  $h$  is used. The updating is still performed using  $d\phi$  to reduce errors due to nonlinearity, but  $d\phi$  is then converted to  $dh$  using a first or second order approximation. The change is necessary because  $h$  can no longer be readily obtained from  $\phi$ .

Occasional iteration of the linear equation solution is required to satisfy certain constraints. A lower limit had to be placed on the estimated time step size reduction to avoid very small

time steps in some situations. Accelerating the time step reduction was helpful in other situations. Note that this iteration to reduce the time step if certain conditions are not obeyed is quite different from the commonly used iterative solution of the original nonlinear balance equations, where fluxes are recalculated each iteration for the same time step until some convergence criterion is satisfied.

Note that solute concentrations in water crossing the bottom boundary are assumed to be equal to those of the water in the bottom layer. If botbc is “constant head” this means that solute may enter the bottom layer from below.

Error messages are directed to the standard output unit (\*). There is very limited checking of parameters. Although messages describe the problem encountered, the cause may not be obvious. For example, bad hydraulic conductivity specification will probably result in the message “getfluxes: too many iterations finding interface h”, indicating that  $h$  at a soil property interface could not be found. Another message that might result from bad property specification is “solve: too many iterations of equation solution”, indicating that the conditions monitored during solution of the approximating equations could not be met. In such situations it may be helpful to use the routine “hyofh” in the property module to produce a list of values of  $S$ ,  $K$  and  $\phi$  for a range of values of  $h$ .

### 4.3. Use of Hydraulic Property Modules

Only those public entities in the hydraulic property modules that are likely to be of direct use are described here. Others are used by the flow module. All are documented in the code.

#### 4.3.1. hypbc

**vars:** derived type whose components are the variables  $h$ ,  $K$ ,  $dK/dS$ ,  $\phi$  and  $d\phi/dS$ , referred to as  $h$ ,  $K$ ,  $KS$ ,  $\phi$  and  $\phi S$ , together with an integer saturation flag  $isat$  (0 when the layer is unsaturated and 1 when it is saturated).

**allo:** subroutine to allocate parameter storage; **call allo (nt, ns)** where  $nt$  and  $ns$  are number of soil types and number of solutes respectively.

**hyofS:** subroutine to get variables  $h$ ,  $K$ ,  $dK/dS$ ,  $\phi$  and  $d\phi/dS$  from  $S$ ; **call hyofS (S, n, jt, var)** where  $S$  is an array of  $n$  saturation values,  $jt$  is an integer array of  $n$  soil type numbers and  $var$  is the array of  $n$  type(vars) variables to be returned. The value of  $isat$  is not altered and variables are returned only where  $S < 1$ .

**hyofh:** subroutine to get variables  $K$ ,  $dK/dh$  and  $\phi$  from  $h$ ; **call hyofh (h, j, K, Kh, phi)** where  $h$  is the head and  $j$  is an integer soil type number.

**Sofh:** function to get degree of saturation  $S$  from matric head  $h$ ; **Sofh (h, j)** where  $h$  is the head and  $j$  is an integer soil type number.

**hypar:** subroutine to set soil hydraulic parameters; **call hypar (j, thr, the, he, Ke, lambda, pp)** where  $j$  is integer soil type number and the other arguments are the BC parameters  $\theta_r$ ,  $\theta_s$ ,  $h_e$ ,  $K_s$ ,  $\lambda$  and  $p$ .

**solpar:** subroutine to set soil solute parameters; **call solpar (j, bdj, disj)** where  $j$  is soil type number,  $bdj$  is soil bulk density and  $disj$  is dispersivity. Bulk density is only used with an adsorption isotherm.

**setiso:** subroutine to set soil solute isotherm type and parameters; **call setiso (j, isol, isotypeji, isoparji)** where  $j$  is integer soil type number,  $isol$  is integer solute number,  $isotypeji$  is a 2 character isotherm code and  $isoparji(:)$  is an array of isotherm parameters. If no isotherm is needed for type  $j$  and solute  $i$ , this routine is not called. A code “li” for linear requires one parameter. If the routine “isosub” provided in the flow module is used, “Fr” requires two parameters, the scaling and the power (in that order), “La” requires the scaling and the shape parameter and “LI” requires the same plus the linear scaling parameter last.

### 4.3.2. hypvgbc

The only difference is in subroutine “hypar”: **call hypar (j, thr, the, hg, Kx, mn, kvg, pp, Kp1, hmac1, Kp2, hmac2, drywrc)** where j, thr and the are as before while hg, Kx, mn, kvg and pp are the real vG water retention and BC conductivity parameters. Kp1, hmac1, Kp2 and hmac2 are optional “macropore” conductivity parameters, with hmac2 < hmac1 if given. The optional logical parameter drywrc, if true, selects the dry soil logarithmic retention curve for  $h < h_{join}$ , where  $h_{join}$  is a parameter set to -15000 cm. The  $b$  parameter in the dry soil conductivity function, Eq. (17), called drypwr, is set to 2. Note that thr must be zero if drywrc is true.

### 4.3.3. hypvgvg

The call to subroutine “hypar”: **call hypar (j, thr, the, hg, Kx, mn, kvg, pp, Ks, drywrc)** is simpler here as macropore component parameters are preset in the module. Ks is the total saturated conductivity and is not optional. Recommended values for  $R_{mac1}$ ,  $h_{mac1}$  and  $h_{mac2}$  of 0.25, -4 and -40 are set as parameters Rmac1, hmac1 and hmac2.

### 4.3.4. Execution times

Execution times for the programs “tstbc”, “tstvgbc” and “tstvgvg” averaged 8, 14 and 15  $\mu$ s per time step respectively (Lahey Fortran 90 Compiler Release 4.00e run on a PC with AMD Athlon™ XP 2400+ 1.99 GHz processor and 512 MB RAM). These times could be reduced by 20% by turning off the compiler switch for array bounds checking. The numbers of time steps required were similar, approximately 220000 for the 729 runs. Thus 200 – 400 such problems could be solved per second.

## 4.4. Approximation for $w$

Ross (2003) gave an approximation for the gravity flux weighting parameter  $w$  for BC hydraulic properties. It was based on  $K(h)$  being a power of  $h$  with index  $-\lambda\eta$  as in Eq. (8). Although  $K(h)$  is not a power of  $h$  near saturation for the other properties, it tends towards one as the soil dries, so that the equivalent approximation for  $w$  can then be used. The BC and vG conductivities of Eqs (9) and (15), combined with the vG retention Eq. (3), do this. By expanding the  $K(h)$  functions in powers of  $x = (h / h_g)^{-n}$ , and retaining only linear terms, we find that  $K(h)$  is proportional to  $x^{m\eta} (1 - \eta mx)$  for the BC form and to  $x^{mp+m+2} [1 - (mp+m+1)x]$  for the vG form. These give the power of  $h$  to use in the approximation, with  $-mn\eta$  for BC and  $-n(mp+m+2)$  for vG, and also the value  $x_e$  of  $x$  at which the absolute relative error in  $K$  is a specified value  $e$ . For the BC conductivity, we have  $\eta mx_e = e$  and for the vG,  $(mp+m+1)x_e = e$ . The parameters  $a$  and  $hpwr$  used in subroutine “weight” are therefore  $mn\eta$  and  $h_g(m\eta / e)^{1/n}$  for BC and  $n(mp+m+2)$  and  $h_g[(mp+m+1) / e]^{1/n}$  for vG.

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