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Scientific Notebook # 343

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LABORATORY NOTEBOOK

CNWRA/SwRI

NOTEBOOK NO. 343

ISSUED TO ILYA S. PARTOM
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INSTRUCTIONS

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2.
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 - Avoid making notes on loose paper to be recycled.
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3.
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 - Record all diagrams, layouts, plans, procedures, new ideas, or anything pertinent to your work including the details of any discussions with suppliers, or other people outside the Company.
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5. Since computer programs can be patented these instructions apply to the development of computer software. In this case a description of the structure and operation of the program should be recorded in the notebook, together with a basic flow diagram which illustrates the essential features of the program. In the course of developing the code, the number of lines of code written each day should be recorded in the notebook, together with a statement of the portion of the flow diagram to which the section of code is directed.
6. This notebook and its contents are the exclusive property of the Company. It is confidential and the contents are not to be disclosed to anyone unless authorized by the Company. You must return it when completed, upon request, or upon termination of employment. It should be kept in a protected place. **If loss occurs, notify your supervisor immediately, and make a written report describing the circumstances of the loss.**

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At the entrance end, we assume that $R(t)$ (rainfall rate) is given. There is enough waste so that the water penetrating to the soil is saturated with radionuclides.

The code will include the following features:

Unsaturated /saturated flow of water.

Transport of dissolved radionuclides.

Transport of colloids.

Movement of colloids from the medium to the water.

Sorption of radionuclides from water by colloids.

Sorption of radionuclides from water by the immobile medium.

At the exit end we monitor the outflow of water and radionuclides. From the breakthrough curves obtained we will (hopefully) deduce transport coefficients.

If we are successful with this, we can then go on to do a similar code for flow and transport in fractures.

General description of the code

COLLOID is a 1D time dependent code that simulates vertical flow of water and transport of radionuclides and colloids in a column of unsaturated/saturated medium.

The code uses finite differences, and the time integration is done explicitly.

We write the code in FORTRAN 90 with DIGITAL FORTRAN.

We divide the column (z direction) into nc equal cells of length dz . We take z positive downwards, where $z=0$ is at ground level.

For each cell along the column we have the following variables:

- $z(i)$ = location of cell upper boundary.
- $v(i)$ = water velocity at cell upper boundary.
- $vnw(i)$ = radionuclides dispersion velocity at cell upper boundary.
- $s(i)$ = degree of saturation, at cell center.

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- $hp(i)$ = pressure head, at cell center.
- $cnw(i)$ = radionuclide concentration in water, at cell center.
- $cns(i)$ = radionuclide concentration in matrix, at cell center.
- $cnwc(i)$ = concentration of radionuclides attached to colloids in water, at cell center.
- $cns(i)$ = concentration of radionuclides attached to colloids in matrix, at cell center.
- $ccw(i)$ = colloid concentration in water, at cell center.
- $ccs(i)$ = colloid concentration in matrix, at cell center.

The units we use for these variables are:

- Time: year (y).
- Length: meter (m).
- Mass: milligram, kilogram (mg), (kg).

The units of the variables above are given at the beginning of the code.

The first thing we do in the code is initializing all the above variable

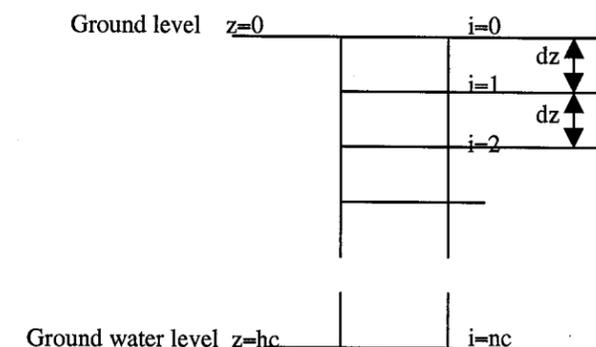


Fig. 1. Column geometry.

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To run the code we also need to input certain fixed data. These are:

- pore = matrix porosity.
- hc = column height.
- dz = cell length.
- dt = integration time increment.
- masb = type of upper boundary condition for the flow. We have (until now three types: 1- constant head; 2- given precipitation rate; 3- finite duration constant head.
- hub = upper boundary head in masb=1 or 3.
- t1 = duration of constant head in masb = 3.
- tmax = maximum running time.
- cnwaq = concentration of radionuclides in the aquifer below the column.
- cnwm = maximum concentration of radionuclides in water.
- cnsm = maximum concentration of radionuclides in matrix.
- ccwout = concentration of colloids in incoming water.
- ccwaq = concentration of colloids in aquifer water.
- ccwm = maximum concentration of colloids in water.
- ccsn = maximum concentration of colloids in matrix.
- tpr = initial output time.
- dtpr = output time step.
- dpor = average pore diameter in the matrix.
- ddn = coefficient of molecular diffusion of radionuclides in water.
- apec, bpec = parameters in effective dispersion versus Peclet number function.

The above fixed data are input to the code by DATA statements. In the future we'll input them from a file using the NAMELIST statement.

The units of the above parameters are given at the beginning of the code.

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To calculate the flow velocities (v) we use Darcy's law.

$$v = -k(s) \left(-1 + \frac{\partial h}{\partial z} \right) \quad (1)$$

where:

s= saturation.

k= hydraulic conductivity.

h= piezometric head.

The -1 term is for the effect of gravity, taking into account that the z axis is positive downwards.

For unsaturated flow $h = -\psi(s)$, where ψ is the suction (negative pressure).

For $\psi(s)$ we use:

$$\psi = \psi_R \left(\frac{s - s_{\min}}{1 - s_{\min}} \right) + \psi_L \left(\frac{1 - s}{1 - s_{\min}} \right) \quad (2)$$

where:

s_{\min} = minimal saturation.

$\psi_R = \psi(1)$.

$\psi_L = \psi(s_{\min})$.

For k(s) we use:

$$k = A(s - s_{\min}) + B(s - s_{\min})^2 \quad (3)$$

The conservation equation for fluid volume is:

$$\frac{\partial s}{\partial t} = - \frac{\partial (sv)}{\partial z} \quad (4)$$

For the dispersion velocity of the nuclides (v_{nw}) use Fick's law:

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$$v_{nw} = -D_{eq} \frac{\partial c_{nw}}{\partial z}$$

where:

D_{eq} = equivalent dispersion coefficient of the radionuclides in the water matrix, and is given by: *(5) 2/15/99 I.P.*

$$D_{eq} = a_{pec} D_d + b_{pec} v d_{av} \quad (6)$$

where:

D_d = molecular diffusion coefficient of the radionuclides in water.

d_{av} = average pore diameter.

a_{pec} , b_{pec} = nondimensional parameters.

For the conservation equation of the radionuclides (ignoring temporarily sorption and decay) we use:

$$\frac{\partial (sc_{nw})}{\partial t} = - \frac{\partial (sv_{nw})}{\partial z} - \frac{\partial (svc_{nw})}{\partial z} \quad (7)$$

For the colloids in water we use the conservation equation (ignoring temporarily retardation effects):

$$\frac{\partial (sc_{cw})}{\partial t} = - \frac{\partial (svc_{cw})}{\partial z} \quad (8)$$

where:

c_{cw} = concentration of colloids in water.

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To take into account the precipitation of colloids on the matrix, we assume that there is equilibrium between the colloids in the water and the colloids in the matrix. This is equivalent to assuming that the time scale to reach equilibrium is much shorter compared to the time scale of colloid transport. The equilibrium equation is:

$$\frac{\rho}{\theta_s} c_{cs} = k_c c_{cw} \quad (9)$$

where θ is the porosity, and k_c is a coefficient to be determined from laboratory tests.

Mass conservation for colloids in the water becomes:

$$\frac{\partial (sc_{cw})}{\partial t} = - \frac{\partial (svc_{cw})}{\partial z} - \frac{\partial (\frac{\rho}{\theta} c_{cs})}{\partial t} \quad (10)$$

Substituting Eq. (9) into Eq. (10) we get:

$$R_c \frac{\partial (sc_{cw})}{\partial t} = - \frac{\partial (svc_{cw})}{\partial z} \quad (11)$$

where:

$$R_c = 1 + k_c \quad (12)$$

and R_c is the retardation factor for the colloids.

To take into account sorption of the radionuclides to the matrix and to the colloids we assume that radionuclide in water, matrix, and on the colloids are in equilibrium.

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The equilibrium equations are:

$$\begin{aligned} \frac{\rho}{\theta_s} c_{ns} &= k_{ns} c_{nw} \\ \frac{\rho}{\theta_s} c_{nsc} &= k_{nsc} c_{nw} \\ c_{nwc} &= k_{nwc} c_{nw} \end{aligned} \quad (13)$$

where k_{ns} , k_{nsc} , and k_{nwc} are the equilibrium coefficients for c_{ns} , c_{nsc} , and c_{nwc} , to be determined from laboratory tests.

The conservation equation for radionuclides in water including sorption and radioactive decay, with a decay coefficient λ is:

$$\begin{aligned} \frac{\partial(sc_{nw})}{\partial t} + \lambda sc_{nw} &= -\frac{\partial(sv_{nw})}{\partial z} - \frac{\partial(svc_{nw})}{\partial z} \\ \left[\frac{\partial(\frac{\rho}{\theta} c_{ns})}{\partial t} + \lambda \frac{\rho}{\theta} c_{ns} \right] &- \left[\frac{\partial(\frac{\rho}{\theta} c_{nsc})}{\partial t} + \lambda \frac{\rho}{\theta} c_{nsc} \right] - \left[\frac{\partial(sc_{nwc})}{\partial t} + \lambda sc_{nwc} \right] \end{aligned} \quad (14)$$

Using Eqs. (13), we get:

$$R_n \frac{\partial(sc_{nw})}{\partial t} = -\frac{\partial(sv_{nw})}{\partial z} - \frac{\partial(svc_{nw})}{\partial z} - \lambda R_n sc_{nw} \quad (15)$$

where R_n is the retardation factor for the radionuclides, and is given by:

$$R_n = 1 + k_{ns} + k_{nsc} + k_{nwc} \quad (16)$$

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The conservation equation for the radionuclides, Eq. (14) above, has something missing. It does not take into account advection of radionuclides attached to colloids in the water. The corrected Eq. (14) reads:

$$\begin{aligned} \frac{\partial(sc_{nw})}{\partial t} + \lambda sc_{nw} &= -\frac{\partial(sv_{nw})}{\partial z} - \frac{\partial(svc_{nw})}{\partial z} - \frac{\partial(svc_{nwc})}{\partial z} \\ \left[\frac{\partial(\frac{\rho}{\theta} c_{ns})}{\partial t} + \lambda \frac{\rho}{\theta} c_{ns} \right] &- \left[\frac{\partial(\frac{\rho}{\theta} c_{nsc})}{\partial t} + \lambda \frac{\rho}{\theta} c_{nsc} \right] - \left[\frac{\partial(sc_{nwc})}{\partial t} + \lambda sc_{nwc} \right] \end{aligned} \quad (17)$$

As a result, Eq. (15) needs also to be corrected. Its corrected version reads:

$$R_n \frac{\partial(sc_{nw})}{\partial t} = -\frac{\partial(sv_{nw})}{\partial z} - R_{nwc} \frac{\partial(svc_{nw})}{\partial z} - \lambda R_n sc_{nw} \quad (18)$$

where:

$$R_{nwc} = 1 + k_{nwc} \quad (19)$$

Description of the COLLOID code.

The code includes several sections. We headline each section with a comment. We now describe the code section by section.

Defining vectors along the column.

We define the vectors using the dimension command. Above that we explain what the vectors are and give their dimensions.

Common /com1/ transfers fixed input data to the functions PSIS and QAYS. These functions evaluate $\psi(s)$ and $k(s)$ respectively.

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Input

We input fixed data using the data command. This is temporary. Later we intend to input fixed data using the namelist command.

Above the data commands we use comments to explain what the data are, and give their dimensions.

Initial conditions

We use a do loop along the column, and input or compute the initial values of the various variables.

Start time march

We start a time march from time=0 to time=tmax with equal increments dt. We use an explicit integration scheme with constant time steps rather than an implicit scheme although this may require smaller time steps. The system is nonlinear, and using an implicit scheme is very complicated.

All the rest of the code is within the time march do loop.

Determine upper boundary head

We provide several options for prescribing the outside head hout. We choose from them using the goto() command, according to the value of masb, which is an input quantity. We now have in the code: masb=1, for constant head, and masb=3, for constant head up to time=t1. We haven't yet implemented masb=2, for given precipitation rate.

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Compute pressure head for saturated sections

We assume that saturated sections may form along the column. In such a case we compute the pressure head in a cell as the distance of the cell center from the upper boundary of the saturated section.

Compute flow velocities

We go along the column with a do loop. In each cell we compute hup and hdn. (We designate by 'up' quantities on the upper side of the cell boundary, and by 'dn' quantities on the lower side of the cell boundary. For unsaturated flow hup=-psiup(sup), and similarly for hdn. The psi(s) relation is evaluated by Eq. (2) in the function PSIS. The relation psi(s) can be easily changed in function PSIS. For saturated flow we use for hup and hdn the piezometric heads computed before.

At the upper boundary we use hup=hout. At the lower boundary we use

hdn=0. *this was corrected later on. I.P. RW 8/15/2000 see at p. 21*

We compute the hydraulic conductivity at a cell boundary using the function QAYS given in Eq. (3). For s we use an effective value seff, given by:

$$s_{eff}(i) = \min(s(i-1), s(i)) \quad (20)$$

Finally we compute the flow velocities by:

$$v(i) = -k \left[-1 + \frac{(h_{dn} - h_{up})}{dz} \right] \quad (21)$$

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Compute radionuclides dispersion velocity

We do this in the same way we compute the flow velocities. We compute cn_{up} and cn_{dn} , where cn is cn_w , the radionuclide concentration in the water. We then compute the equivalent dispersion coefficient D_{eq} by Eq. (6), and the dispersion velocities by:

$$v_{nw}(i) = -D_{eq} \frac{(cn)_{dn} - (cn)_{up}}{dz} \quad (22)$$

At the upper boundary we use $cn_{up} = cn_{wm}$, which is the maximum concentration of radionuclides in water. At the lower boundary we use $cn_{dn} = 0$.

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Computing new saturations

To compute the new saturations from water volume conservation, we first calculate the products vs_{up} and vs_{dn} . vs_{up} for cell i is either $v(i) * s(i-1)$, or $v(i) * s(i)$, depending on flow direction. Similarly, vs_{dn} is either $v(i+1) * s(i)$ or $v(i+1) * s(i+1)$. For the upper and lower boundaries ($i=1$, and $i=nc+1$) we use $s=1$ when the flow is into the column.

We then calculate the new saturations from the volume conservation equation in finite differences as follows:

$$s_{new}(i) = s(i) + \frac{dt}{dz} (vs_{up} - vs_{dn}) \quad (23)$$

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Computing new radionuclides concentrations

Similar to the quantities vs_{up} and vs_{dn} above, we first compute here the quantities vsc_{up} , vsc_{dn} , vnw_{sup} , and vnw_{sdn} . vsc_{up} is either $v(i) * s(i-1) * cn_w(i-1)$, or $v(i) * s(i-1) * cn_w(i-1)$, depending on the flow direction, and similarly with vsc_{dn} . vnw_{sup} is either $vnw(i) * s(i-1)$ or $vnw(i) * s(i)$, and similarly for vnw_{sdn} , depending on the dispersion direction. At the upper and lower boundaries we use $cn_w(i-1) = cn_{wm}$, and $cn_w(nc+1) = 0$, when the flow is into the column.

We then use conservation of radionuclides mass in finite differences to compute the new radionuclides concentrations.

$$cn_{w_{new}}(i) = \frac{1}{s_{new}(i)} cn_w(i) s(i) + \frac{1}{s_{new}(i)} \frac{dt}{dz} \frac{1}{R_n} [R_{nwc} (vsc_{up} - vsc_{dn}) + (vnw_{sup} - vnw_{sdn})] - \lambda s(i) cn_w(i) \quad (24)$$

R_n and R_{nwc} enter into this equation as explained above with respect to Eqs. (18), and (19).

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Computing new colloid concentrations

Similar to radionuclides above, we compute vsc_{up} and vsc_{dn} at the upper and lower cell boundaries by. vsc_{up} is either $v(i) * s(i-1) * ccw(i-1)$ or $v(i) * s(i) * ccw(i)$, and vsc_{dn} is either $v(i+1) * s(i) * ccw(i)$ or $v(i+1) * s(i+1) * ccw(i+1)$, depending on the flow direction. At the upper boundary we use $s=1$ and $ccw(i-1) = ccw_{out}$, and at the lower boundary we use $s=1$ and $ccw(i+1) = ccw_{aq}$, when the flow direction is into the column.

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We compute the new colloid concentrations using the conservation equation for the colloids in water. In finite differences it reads:

$$ccw_{new}(i) = \frac{1}{s_{new}(i)} \left[ccw(i)s(i) + \frac{1}{R_c} \frac{dt}{dz} (v_{sc_{up}} - v_{sc_{dn}}) \right] \quad (25)$$

R_c is the retardation coefficient for the colloids, as defined in Eq. (12).

Avoiding numerical dispersion for saturation, radionuclides concentrations, and colloid concentrations.

Whenever the absolute change in saturation in a cell is less than ϵs_s , we transfer that change to the uppermost cell.

We then correct the new concentrations in the uppermost cell accordingly.

Whenever the absolute change in Radionuclides or colloids concentrations in a cell is less than ϵs_n , or ϵs_c , respectively, we transfer the changes to the uppermost cell.

Adjusting for $s > 1$ and $s < s_{min}$.

Whenever $s_{new}(i) > s_{sat}$, and $s_{new}(i+1) < 1$, we set $s_{new}(i)$ to s_{sat} , and transfer the difference to the cell below. s_{sat} is a value slightly lower than 1. We use $s_{sat} = 0.999$.

Whenever $s_{new}(i) > 1$, $s_{new}(i+1) = 1$, we set $s_{new}(i)$ to 1, and transfer the difference to the cell below.

In this way we ensure that the column can become saturated only from the aquifer upwards, and not from the upper boundary downwards.

Whenever $s_{new}(i) > 1$, $s_{new}(i+1) = 1$, we set $s_{new}(i)$ to 1, and transfer the difference to the cell below.

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In this way we ensure that the column can become saturated only from the aquifer upwards, and not from the upper boundary downwards.

Whenever $s_{new}(i) < s_{min}$, we set $s_{new}(i)$ to s_{min} , and transfer the difference to the cell above.

In both cases, we correct the radionuclides concentration and the colloid concentration in the receiving cells accordingly.

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Updating s, cnw, and ccw along the column

After all the corrections and adjustments, we put the new values $s_{new}(i)$, $cnw_{new}(i)$ and $ccw_{new}(i)$, into the old values $s(i)$, $cnw(i)$ and $ccw(i)$.

Computing accumulated mass of radionuclides and of colloids outflowing through a chosen cell boundary

We designate the chosen cell boundary as $i=iac$. The outflowing colloid mass during the time dt is given by: $\theta v(i)s(i-1)ccw(i-1)dt$ or $\theta v(i)s(i)ccw(i)dt$, depending on the flow direction. The outflowing radionuclides mass during the time dt is the sum of convection flow and dispersion flow. Convection flow is given by: $\theta v(i)s(i-1)cnw(i-1)dt$ or $\theta v(i)s(i)cnw(i)dt$. Dispersion flow is given by: $\theta v_{nw}(i)s(i-1)dt$ or $\theta v_{nw}(i)s(i)dt$, depending on the dispersion flow direction.

We accumulate the outflowing colloid mass in scw , and the outflowing radionuclides mass in $scnw$.

We're now ready to output the results of this time cycle and to start a new cycle.

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All the information below has been taken from: NRC Iterative Performance Assessment Phase 2.

Table-1:

	Grain density (Kg/m**3)	Porosity	Residual saturation	Saturated Conductivity (mm/yr)	Alpha (1/m)	Beta
Topopa Spring w. Calico Hills n.w.v	2580.	.06 -.16	.080	.11 - 36.	.006	1.4 - 2.2
Calico Hills n.w.z	2370.	.33 -.56	.041	1.2E2 - 6.1E3	.016	1.5 - 4.9
Calico Hills n.w.z	2230.	.20 -.33	.110	.004 - .20	.003	1.2 - 3.3
Prow Pass, w.	2590.	.24 -.40	.066	58. - 300.	.014	2.0 - 3.4
U&M Crater Flat, non-w.	2270.	.18 - .30	.135-.322 U	1.6 - 4.6 Up. 1.3 - 4.8 Md.	.004	1.5 - 2.4
Bullfrog, Welded.	2630.	.19-.32	.056 - .061	110. - 140.	.02	2.3 - 4.2

The Grain Density, Porosity, Saturated Conductivity, Alpha and Beta are copied from Table B-6, page B-24. The Residual Saturation are taken from Table B-1, pp. B-2 - B-9.

Table - 2: K_d (m**3/kg)

Element	Topopa Spring	Calico Hills n.w.v	Calico Hills n.w.z	Prow Pass	Up. & Md. Crater Flat	Bullfrog
Am	.810	.810	1.7	4.5	1.36	.140
Pu	.170	.170	.066	.130	.053	.094
U	.0002	.020	.001	0.0	.0008	.002
Se	.0026	.003	.0045	.0025	.0036	.013
Tc	1.3e-5	0.0	0.0	1.7E-4	----	.0042
Np	.0045	.0045	.0027	.0051	.0022	.0051
Sr	.08	.034	8.9	.450	7.1	.280
Cs	.36	.24	22.0	2.2	17.6	3.2
Ba	1.2	.6	61.0	3.9	-----	1.1
Ra	1.5	1.5	1.5	1.5	1.2	5.0

This Table has been copied from page B-16, and table B-7 page B-26

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The Genuchten equations are page 4-27 and page 4-28:

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$$s = (s_s - s_r) \left[\frac{1}{1 + |\alpha h|^\beta} \right]^{(1-\frac{1}{\beta})} \quad (1)$$

and

$$k_r = \left[1 - \left(1 - (s_e)^\lambda \right)^2 \right] \sqrt{s_e} \quad (2)$$

Where: s = saturation.

s_s = saturation at full saturation.

s_r = residual saturation.

h = pressure or suction.

α, β = fitting parameters.

k_r = relative conductivity.

λ = van Genuchten fitting parameter (1-1/ β)

s_e = effective saturation given by:

$$s_e = \frac{s - s_r}{s_s - s_r} \quad (3)$$

The retardation factor R_f is calculate from the distribution coefficient (k_d) (page 4-30) by:

$$R_f = 1 + \frac{\rho(1-n)}{\theta} k_d \quad (4)$$

Where: θ = moisture content.

ρ = grain density.

n = porosity.

In page 4-53 we find "The system code uses of the present NCR performance assesment uses the k_d approach in estimating retardation of radionuclides. The relationship of k_d to retardation is:

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$$R_f = 1 + \rho \frac{k_d}{\theta} \quad (5)$$

From what is written in Appendix B, comes that after all eq.(4) is the one that was used.

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We wanted to use Van-Genuchten functions for $\psi(s)$ and $k(s)$. We first evaluated those functions for some values of the parameters α and β , with the help of a code built for VG equations and given below.

```

! Code for calculating the saturation (s),and the hydraulic
! conductivity from the VG equatins.

! s= saturation.
! ss= saturation at at full saturation.
! sr= residual saturation.
! h= pressure or suction (m).
! alfa= fitting parameter (1/m).
! beta= fitting parameter.
! kr= relative conductivity.
! ksat= saturated conductivity (m/yr).
! k= conductivity at given saturation (m/yr).

data ss,sr/.999,.08/
data alfa,beta/.006,1.8/
data hmax/1000./
data qsat/1.0e-3/

elamda=1.-1./beta
dh=hmax/20.

do h=hmax,dh,-dh
s=(ss-sr)*(1./(1.+(abs(alfa*h)**beta)**elamda)
print *,h,s
seff=(s-sr)/(ss-sr)
qr=(1.-(1.-seff**(1./elamda))**elamda)**2*sqrt(seff)
q=qr*qsat
if(s.le.sr) goto 999
write (1,*) h,s,seff,qr,q
enddo

999 end

```

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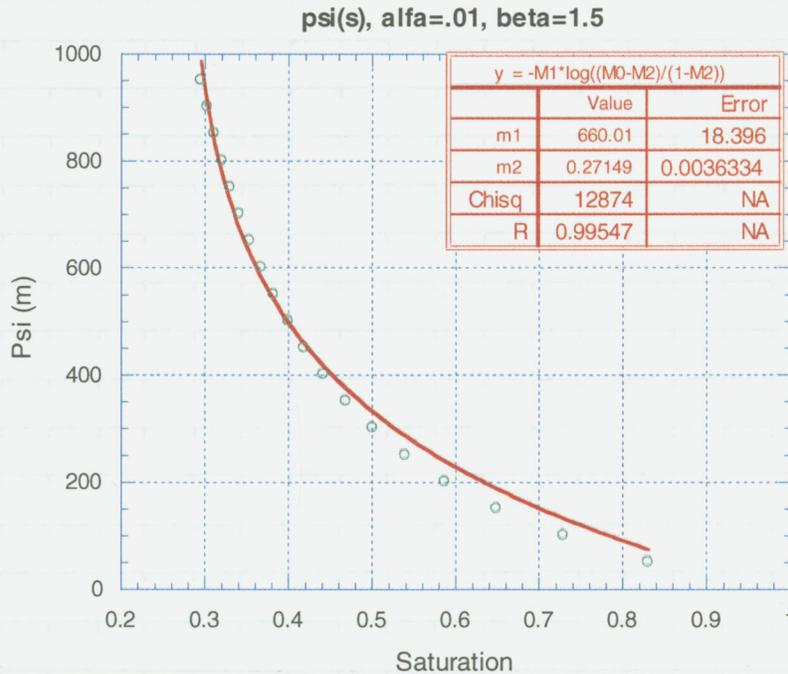
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We saw that $\psi(s)$ is not defined for values of s close to 1. Because our code is intended for both saturated and unsaturated flow, we need $\psi(s)$ to be defined for all s . We therefore plotted $\psi(s)$ and $k(s)$, and curvefitted them with simple functions. The functions are:

$$\psi = -\psi_0 \ln \frac{s - s_1}{1 - s_1} \tag{26}$$

$$k = a_0 + a_1s + a_2s^2 + a_3s^3 + a_4s^4$$

For $\alpha=0.01/m$, $\beta=1.5$ the, $s_{min}=0.08$, $s_{sat}=0.999$, $k_{sat}=.001$ m/y the Van-Genutchen and the curve fits are given below.



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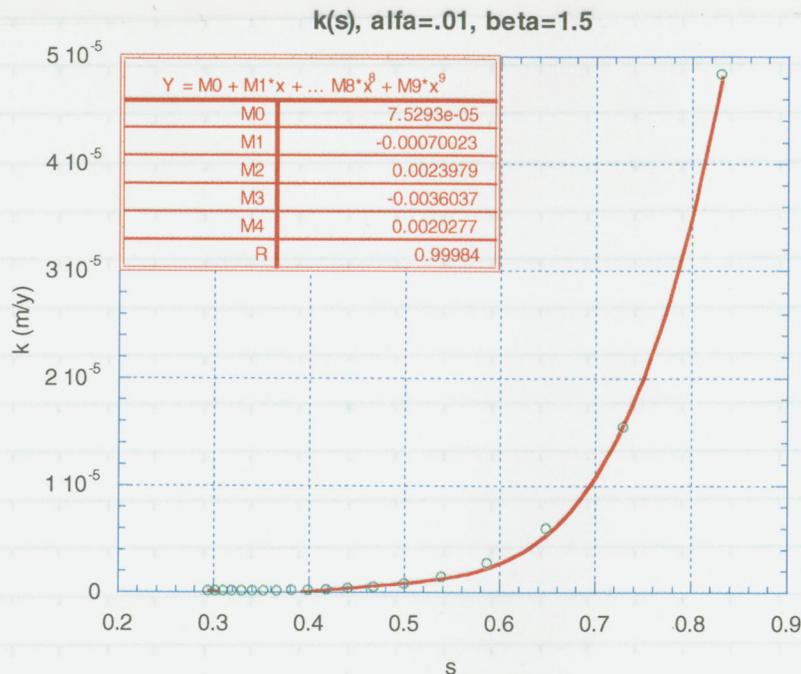
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*Skolmm
2/7/00*

We intend to use equations (26) for $\psi(s)$ and $k(s)$ in the code as `maspsik=3`.

We introduced the reading in of input data through the NAMELIST command. This is convenient because the NAMELIST file is written in free format in the form: `a=####`, `b=####`, etc. The input file is `fort.11`. On file `fort.12` we print out all the data input from `fort.11`.

*Skolmm
2/7/00*

To be able to identify which input data was used to obtain certain output data, we introduce a sequential run number denoted by `nrun`. At the beginning of a run we read the previous `nrun` from `fort.13` and rewind `fort.13`. We then write `nrun` on all output files. At the end of the run we increase `nrun` by 1, and write the new `nrun` on `fort.13`.

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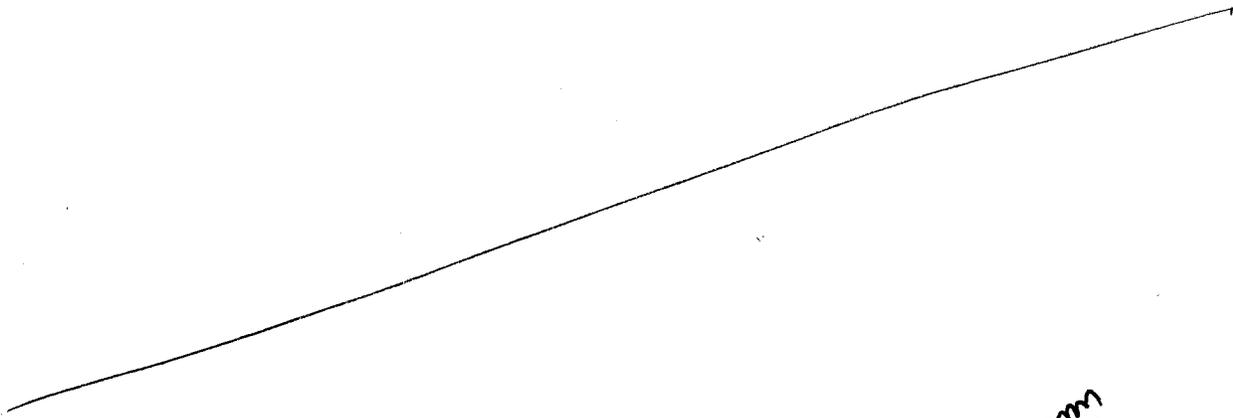
7/29/1999

To observe the effect of colloids on the transport of radionuclides, we introduced a mass accumulation scheme. We input the parameter i_{ac} , which is the number of the cell boundary through which we accumulate the mass of radionuclides and the mass of colloids. Radionuclides going through a cell boundary come from three sources: convected with the water, convected with colloids in the water, and dispersed relative to the flow. At each time step we calculate the rates of these three components, multiply by dt and add to the accumulated mass obtained at the previous time. We do the same for the colloids in the water. We printout the accumulated mass values on file 2.

When the flow reaches the lower boundary (aquifer level), the column becomes saturated from the bottom up. This means that the phreatic level (interface between the saturated and the unsaturated zones) rises. But in a real situation the phreatic level would not rise so fast because of radial flow in the aquifer (which are not included in our model). To account for the radial effect we adjusted the lower boundary condition as follows. When the phreatic level rises by Δh , we apply a velocity boundary condition, and the velocity is given by:

$$v(nc + 1) = \alpha_{aq} \Delta h \quad (27)$$

where α_{aq} is an input coefficient. The effect of this boundary condition is to slow down the rise of the phreatic level.



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We introduced a velocity boundary condition for the flow at the upper boundary. We prepared space for it before, and we called it masb=2 (see above). According to this boundary condition the inflow velocity is v_{in} during $0 < t < t_2$ at the beginning of each year, and $v_{in}=0$ for the rest of the year. The input parameters for this boundary condition are v_{in} and t_2 .

Initially we didn't limit the amount of radionuclides that could be adsorped to the colloid particles in the water, assuming that the concentration of colloids was always large enough. But to be able to reduce the colloid concentration down to zero, we introduced a saturation limit for the adsorped radionuclides. We added an input parameter denoted by α_n . The concentration limit is given by:

$$(c_{nwc})_m = \alpha_n c_{cw} \quad (28)$$

We see that the saturation limit is different for each cell. When c_{nwc} reaches the saturation limit there is no more in equilibrium with the radionuclides in the water, and the conservation equation for the radionuclides has to be changed. We change it as follows:

- We go back to Eq. (17).
- Wherever old values are used in the finite difference equivalent of Eq. (17), we use the known values of c_{nwc} .
- For the new values of c_{nwc} we use a two step procedure.
- In step one we assume equilibrium.
- In step two we check if the saturation limit has been passed. If it has, we set c_{nwc} to $\alpha_n c_{cw}$ and adjust c_{nw} accordingly.

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COLLOID

Movement of water, radionuclids and colloids iv a vertical unsaturated column.
1D time dependent code.

z= vertical location measured downward (m).
s= degree of saturation.
snew= degree of saturation at end of time step.
v= fluid velocity (m/y).
hp= pressure head (m).
cnw= mass of radionuclides in water per unit volume of fluid (mg/m**3).
cnwnew= mass of radionuclides in water per unit volume of fluid at end of time step (mg/m**3).
ccwnew= mass of colloids in water per unit volume of fluid at end of time step (mg/m**3).
cns= mass of radionuclides sorbed in non colloidal matrix per unit matrix mass (mg/kg).
cnsc= mass of radionuclides sorbed on colloids in matrix per unit matrix mass (mg/kg).
cnwc= mass of radionuclides sorbed on colloids in water per unit volume of fluid (mg/m**3).
ccs= mass of colloids in matrix per unit matrix mass (mg/kg).
ccw= mass of colloids in water per unit volume of fluid (mg/m**3).
vbw= dispersion velocity of radionuclides in water (mg/m**2/y).
cell bounary i is above cell i.
s, hp, c... defined in cell.
z, v, vbw defined at cell boundary.
common/com1/ssat, smin
common/com12/maspsik
common/com2/alfa, beta, gamma, qaysat
common/psi20/psi0, s1
dimension z(500), s(500), snew(500), v(500), hp(500)
dimension cnw(500), cns(500), ccs(500), ccw(500), cnwc(500), cnsc(500)
dimension cnwnew(500), ccwnew(500)
dimension vbw(500)

INPUT

teta= porosity of matrix (volume of pores per unit volume).
ro= density of the matrix (kg/m**3).
hc= column height (m).
dz= cell size (m).
dt= time step (y).
tmax= maximum runningtime (y).
cnwaq= mass of radionuclides in water per unit volume of aquifer water (mg/m**3).
cnwm= maximum mass of radionuclides in water per unit volume of fluid (mg/m**3).
ccwout= concentration of colloids in incoming water (mg/m**3).
ccwaq= concentration of colloids in aquifer water.
sint= initial saturation.
ccwint= initial concentration of colloids in water (mg/m**3).
cnwint= initial concentration of nuclides in water (mg/m**3).
masb= flow boundary contition type. masb=1: constant head. masb=2: given precipitation rate.
masb=3: constant head up to t=t1.
hub= upper boundary given constnt head in masb=1,3 (m).
t1= duration of constant head in masb=3.
t21= biginning of irrigation period in masb=2.
t22= end of irrigation period in masb=2.
t23=biginning of anew irrigation period in masb=2.
tpr=initial output time (y).
dtp= printing time step (y).
dp= average tetae diameter of porous medium (m).
ddn= molecular diffusion coefficient for the radionuclides (m**2/y).
ibt= number of cell for breakthrough curve.
apec, bpec= parametersin effective dispersionversus Peclet number function.
rc=retardation function for colloids.
rn=retardation function for nuclides.
qayd=absorption coefficient (m**3/kg)
elamda=radioactive decay coefficient (1/y).
virrig=annual irrigation (m/y)
consaq= A constant for calculating v(nc+1) when the phriatic surface rises.
The equation is: v(nc+1)=consaq*dh where dh is the rise of the phriatic surface level (1/y).
alfan=a non dimensional coeff. determaning the capacity of the colloid to absorb nuclides, used in function: cnwc=alfan*ccw(i).

namelist/in/nrun
namelist/in/teta, ro, cnwm, ccwout, qaysat
namelist/in/sint, ccwint, cnwint, masb, maspsik, hub, t1
namelist/in/t21, t22, t23, virrig, consaq
namelist/in/epss, epsnw, epscw, ssat, smin, ccwaq, cnwaq
namelist/in/dp, apec, bpec, ddn, rc, elamda, ibt, iac
namelist/in/alfa, beta, psi0, s1, qayd, ckdns, ckdnsc, ckdnc, alfan
namelist/in/hc, dz, dt, tmax, tpr, dtpr

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```

data nrun/1/
data teta,ro/.3,2000./
data hc,dz/300.,10./
data dt,tmax/1.,50./
data tpr,dtpr/0.,1./
data hub,t1/.01,10000./
data t21,t22,t23,virrig/0.,.5,1.,.76/
data cnwm,ccwout/2.4,1.e4/
data sint,ccwint,cnwint/.7,5.e3,0./
data masb,maspsik/3,2/
data dpor,ddn/1.e-4,.038/
data apec,bpec/.63,1./
data epss,epsnw,epscw/1.e-6,1.e-5,1.e-6/
data smin,ssat/.25,.99/
data ccwaq,cnwaq,consaq/.1,0.,.25/
data rc,qayd,elamda/1.0,4.e3,0./
data ibt/5/
data iac/5/
data alfa,beta,qaysat/.016,1.3,10./
data psi0,s1/66.,.4/
data ckdns,ckdnsc,ckdnwc,alfan/0.,0.,1.,2.4e-4/

```

```

write(11,*)
write(13,*)
read(11,in)
read(13,*)nrun
rewind 13
write(12,in)

```

nc= number of cells in column.

INITIAL CONDITIONS

```

deldt=dt/100.
scw=0.
scnw=0.
scnwc=0.
qayc=rc-1.
qayn=qayd*teta/ro
qayns=ckdns*qayn
qaynsc=ckdnsc*qayn
qaynwc=ckdnwc*qayn
rn=1.+qayn
rn=1.+qaynwc+qayns+qaynsc
gamma=1.-1./beta
nc=hc/dz
cnwcout=min(qaynwc*cnwm,alfan*ccwout)
cnwcaq=min(qaynwc*cnwaq,alfan*ccwout)
do i=1,nc
s(i)=sint
z(i)=(i-1)*dz
cnw(i)=cnwint
ccw(i)=ccwint
cns(i)=teta/ro*qayns*cnw(i)*s(i)
cnsc(i)=teta/ro*qaynsc*cnw(i)*s(i)
cnwc(i)=qaynwc*cnw(i)
ccs(i)=teta/ro*qayc*ccw(i)*s(i)
enddo
z(nc+1)=hc
s(nc+1)=1.

```

header output

```

write (1,111),nrun
write (3,131),nrun,ccwint,rc
write (2,121),nrun,ibt,iac
write (2,122) rn,qayns,qaynsc,qaynwc,rc
write (2,123)

```

START TIME MARCH

```

do time=dt,tmax,dt

```

determine upper boundary head.

```

goto (10,20,30) masb

```

masb=1, constant head.

```

10 continue
hout=hub
vin=0.
t1=tmax+dt
goto 11

```

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20 masb=2, given precipitation rate.
continue
hout=0.
if(time.ge.t21.and.time.lt.t22) vin=virrig
if(time.ge.t22.and.time.lt.t23) vin=0.
if(time.gt.t23) then
t21=t21+1.
t22=t22+1.
t23=t23+1.
vin=virrig
endif
goto 11

30 masb=3, hout=hub until t=t1, then hout=0.
continue
if(time.lt.t1) then
hout=hub
else
hout=0.
vin=0.
endif
goto 11
continue

11 compute pressure head for saturated sections.
zsat=0.
isat=1
flag=0.
do i=1,nc+1
if(flag.eq.0.and.s(i).eq.1.) then
flag=1.
hsat=z(i)
endif
if(s(i).lt.1.) then
hp(i)=0.
zsat=z(i+1)
isat=i+1
else
hp(i)=z(i)+.5*dz-zsat
endif
enddo

compute flow velocities
do i=1,nc+1
if(i.eq.1) then
sup=1.
hup=hout
else
sup=s(i-1)
psiup=psis(sup)
if(sup.lt.1.) then
hup=-psiup
else
hup=hp(i-1)
endif
endif
if(i.eq.nc+1) then
sdn=1.
hdn=hp(nc+1)
else
sdn=s(i)
psidn=psis(sdn)
if(sdn.lt.1.) then
hdn=-psidn
else
hdn=hp(i)
endif
endif
seff=min(sup,sdn)
qay=qays(seff)
if(i.eq.1.and.hout.eq.0.) then
v(1)=vin
else
v(i)=-qay*(-1.+(hdn-hup)/dz)
endif
enddo

vout=consaq*(hc-zsat)
vout=min(vout,qaysat)

```

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do i=isat,nc+1
v(i)=vout
enddo

compute radionuclides dispersion velocities.
do i=1,nc+1
if(i.eq.1) then
cnp=cnmw
else
cnp=cnw(i-1)
endif
if(i.eq.nc+1) then
cnd=cnwaq
else
cnd=cnw(i)
endif
pecle=abs(v(i))*dpor/ddn
deq=ddn*apec
deqn=ddn*apec*(1.+pecle/bpec)
vnw(i)=-deq*(cnd-cnp)/dz
enddo

computing new saturations.
do i=1,nc
if(i.eq.1) then
if(v(1).ge.0.) then
vsup=v(1)*1.
else
vsup=v(1)*s(1)
endif
if(v(2).ge.0.) then
vsdn=v(2)*s(1)
else
vsdn=v(2)*s(2)
endif
endif

if(i.gt.1.and.i.lt.nc) then
if(v(i).ge.0.) then
vsup=v(i)*s(i-1)
else
vsup=v(i)*s(i)
endif
if(v(i+1).ge.0.) then
vsdn=v(i+1)*s(i)
else
vsdn=v(i+1)*s(i+1)
endif
endif

if(i.eq.nc) then
if(v(i).ge.0.) then
vsup=v(i)*s(i-1)
else
vsup=v(i)*s(i)
endif
if(v(i+1).ge.0.) then
vsdn=v(i+1)*s(i)
else
vsdn=v(i+1)*1.
endif
endif
snew(i)=s(i)+dt/dz*(vsup-vsdn)
enddo

computing new radionuclides concentrations.
do i=1,nc
if(i.eq.1) then
if(v(1).ge.0.) then
vscup=v(1)*1.*cnwm
vsccup=v(1)*1.*cnwcout
else
vscup=v(1)*s(1)*cnw(1)
vsccup=v(1)*s(1)*cnwc(1)
endif
if(v(2).ge.0.) then
vsdcn=v(2)*s(1)*cnw(1)
vsccdn=v(2)*s(1)*cnwc(1)
else
vsdcn=v(2)*s(2)*cnw(2)

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vsccdn=v(2)*s(2)*cnwc(2)
endif
if(vnw(1).gt.0.) then
vnwsup=vnw(1)*1.
else
vnwsup=vnw(1)*s(1)
endif
if(vnw(2).ge.0.) then
vnwsdn=vnw(2)*s(1)
else
vnwsdn=vnw(2)*s(2)
endif
endif

if(i.gt.1.and.i.lt.nc) then
if(v(i).ge.0.) then
vscup=v(i)*s(i-1)*cnw(i-1)
vsccup=v(i)*s(i-1)*cnwc(i-1)
else
vscup=v(i)*s(i)*cnw(i)
vsccup=v(i)*s(i)*cnwc(i)
endif
if(v(i+1).ge.0.) then
vsdcn=v(i+1)*s(i)*cnw(i)
vsccdn=v(i+1)*s(i)*cnwc(i)
else
vsdcn=v(i+1)*s(i+1)*cnw(i+1)
vsccdn=v(i+1)*s(i+1)*cnwc(i+1)
endif
if(vnw(i).ge.0.) then
vnwsup=vnw(i)*s(i-1)
else
vnwsup=vnw(i)*s(i)
endif
if(vnw(i+1).ge.0.) then
vnwsdn=vnw(i+1)*s(i)
else
vnwsdn=vnw(i+1)*s(i+1)
endif
endif

if(i.eq.nc) then
if(v(i).ge.0.) then
vscup=v(i)*s(i-1)*cnw(i-1)
vsccup=v(i)*s(i-1)*cnwc(i-1)
else
vscup=v(i)*s(i)*cnw(i)
vsccup=v(i)*s(i)*cnwc(i-1)
endif
if(v(i+1).ge.0.) then
vsdcn=v(i+1)*s(i)*cnw(i)
vsccdn=v(i+1)*s(i)*cnwc(i)
else
vsdcn=v(i+1)*1.*cnwcaq
vsccdn=v(i+1)*1.*cnwcaq
endif
if(vnw(i).ge.0.) then
vnwsup=vnw(i)*s(i-1)
else
vnwsup=vnw(i)*s(i)
endif
if(vnw(i+1).ge.0.) then
vnwsdn=vnw(i+1)*s(i)
else
vnwsdn=vnw(i+1)*1.
endif
endif
cnwnew(i)=((cnw(i)*(1.+qayns+qaynsc)+cnwc(i))*s(i)/rn+dt/dz*(vscup-vsdcn+vsccup-vsccdn
& +vnwsup-vnwsdn)/rn-elamda*s(i)*dt/rn*(cnw(i)*(1.+qayns+qaynsc)+cnwc(i)))/snew(i)
enddo

computing new colloids concentrations.
do i=1,nc
if(i.eq.1) then
if(v(1).ge.0.) then
vscup=v(1)*1.*ccwout
else
vscup=v(1)*s(1)*ccw(1)
endif
if(v(2).ge.0.) then

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vscdn=v(2)*s(1)*ccw(1)
else
vscdn=v(2)*s(2)*ccw(2)
endif
endif

if(i.gt.1.and.i.lt.nc) then
if(v(i).ge.0.) then
vscup=v(i)*s(i-1)*ccw(i-1)
else
vscup=v(i)*s(i)*ccw(i)
endif
if(v(i+1).ge.0.) then
vscdn=v(i+1)*s(i)*ccw(i)
else
vscdn=v(i+1)*s(i+1)*ccw(i+1)
endif
endif

if(i.eq.nc) then
if(v(i).ge.0.) then
vscup=v(i)*s(i-1)*ccw(i-1)
else
vscup=v(i)*s(i)*ccw(i)
endif
if(v(i+1).ge.0.) then
vscdn=v(i+1)*s(i)*ccw(i)
else
vscdn=v(i+1)*1.*ccw(i)*ccwaq
endif
endif
ccwnew(i)=(ccw(i)*s(i)+dt/dz*(vscup-vscdn)/rc)/snew(i)
enddo

avoiding numerical dispersion in s.
do i=2,nc
if(abs(snew(i)-s(i)).lt.epss) then
dels=snew(i)-s(i)
ccwnew(1)=(ccwnew(1)*snew(1)+dels*ccwnew(i))/(snew(1)+dels)
cnwnew(1)=(cnwnew(1)*snew(1)+dels*cnwnew(i))/(snew(1)+dels)
snew(i)=s(i)
snew(1)=snew(1)+dels
endif
enddo

adjusting for s(i)>1.
do i=1,nc-1
if(snew(i).gt.ssat.and.s(i+1).lt.1.) then
dels=snew(i)-ssat
ccwnew(i+1)=(ccwnew(i+1)*snew(i+1)+dels*ccwnew(i))/(snew(i+1)+dels)
cnwnew(i+1)=(cnwnew(i+1)*snew(i+1)+dels*cnwnew(i))/(snew(i+1)+dels)
snew(i+1)=snew(i+1)+dels
snew(i)=ssat
endif
if(snew(i).gt.1.and.s(i+1).eq.1.) then
dels=snew(i)-1.
ccwnew(i+1)=(ccwnew(i+1)*snew(i+1)+dels*ccwnew(i))/(snew(i+1)+dels)
cnwnew(i+1)=(cnwnew(i+1)*snew(i+1)+dels*cnwnew(i))/(snew(i+1)+dels)
snew(i+1)=snew(i+1)+dels
snew(i)=1.
endif
enddo
if(snew(nc).gt.1.) snew(nc)=1.

adjusting for s(i)<smin.
do i=nc,2,-1
if(snew(i).lt.smin) then
dels=snew(i)-smin
ccwnew(i-1)=(ccwnew(i-1)*snew(i-1)+dels*ccwnew(i))/(snew(i-1)+dels)
cnwnew(i-1)=(cnwnew(i-1)*snew(i-1)+dels*cnwnew(i))/(snew(i-1)+dels)
snew(i-1)=snew(i-1)+dels
snew(i)=smin
endif
enddo
if(snew(1).lt.smin) snew(1)=smin

avoiding numerical dispersion for nuclides.
do i=2,nc
if(abs(cnwnew(i)-cnw(i)).lt.epsnw) then
delnw=cnwnew(i)-cnw(i)

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cnwnew(i)=cnw(i)
cnwnew(1)=cnwnew(1)+delnw*snew(i)/snew(1)
endif
enddo
if(abs(cnwnew(1)-cnw(1)).lt.epsnw) cnwnew(1)=cnw(1)

adjusting for cnw>cnwm.
do i=1,nc
if(cnwnew(i).gt.cnwm) then
cnwnew(i)=cnwm
endif
enddo

avoiding numerical dispersion for colloids.
do i=2,nc
if(abs(ccwnew(i)-ccw(i)).lt.epscw) then
delcw=ccwnew(i)-ccw(i)
ccwnew(i)=ccw(i)
ccwnew(1)=ccwnew(1)+delcw*snew(i)/snew(1)
endif
enddo
if(abs(ccwnew(1)-ccw(1)).lt.epscw) ccwnew(1)=ccw(1)

computing mass of colloids and nuclides accumulating at i=iac
i=iac
if(v(i).gt.0.) then
sccw=sccw+teta*s(i-1)*ccw(i-1)*v(i)*dt
scnwc=scnwc+teta*s(i-1)*cnwc(i-1)*v(i)*dt
if(vnw(i).gt.0.) then
scnd=teta*vnw(i)*s(i-1)
else
scnd=teta*vnw(i)*s(i)
endif
scnw=scnw+(teta*s(i-1)*cnw(i-1)*v(i)+scnd)*dt
sntot=scnwc+scnw
else
sccw=sccw+teta*s(i)*ccw(i)*v(i)*dt
scnwc=scnwc+teta*s(i)*cnwc(i)*v(i)*dt
if(vnw(i).gt.0.) then
scnd=teta*vnw(i)*s(i-1)
else
scnd=teta*vnw(i)*s(i)
endif
scnw=scnw+(teta*s(i)*cnw(i)*v(i)+scnd)*dt
sntot=scnwc+scnw
endif

update saturations.
do i=1,nc
s(i)=snew(i)
enddo

update nuclides concentrations in water (cnw).
do i=1,nc
cnw(i)=cnwnew(i)
enddo

update colloids concentrations in water (cnw).
do i=1,nc
ccw(i)=ccwnew(i)
enddo

computing of radionuclides mass sorbed on non colloidal matrix, on
colloids in matrix, on colloids in water, and of mass of colloids in matrix,
and correcting for saturation of amount of nuclides sorped to colloids in the water.
do i=1,nc
cns(i)=teta/ro*qayns*cnw(i)*s(i)
cnsc(i)=teta/ro*qaynsc*cnw(i)*s(i)
cnwc(i)=qaynwc*cnw(i)
ccs(i)=teta/ro*qayc*ccw(i)*s(i)

cnwcm=alfan*ccw(i)
if(cnwc(i).gt.cnwcm) then
delcnwc=cnwc(i)-cnwcm
cnwc(i)=cnwcm
delcnw=delcnwc/(1.+qayns+qaynsc)
cnw(i)=cnw(i)+delcnw
if(cnw(i).gt.cnwm) cnw(i)=cnwm
cns(i)=cns(i)+teta/ro*s(i)*qayns*delcnw

```

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Recorded by

2/21/70

```
cnsc(i)=cnsc(i)+teta/ro*s(i)*qaynsc*delcnw
endif
```

```
enddo
```

```
output.
```

```
if(time.ge.(tpr-deldt))then
write (1,113)tpr,zsat
write (3,133)tpr,zsat
write (1,112)
write (3,132)
tpr=tpr+dtpr
do i=1,nc+1
write(1,114) z(i),s(i),v(i),vnw(i),cnw(i)
write(3,134) z(i),s(i),v(i),ccw(i)
enddo
write(2,124)time,cnw(ibt),scnw,scnwc,sntot,sccw
endif
```

```
END TIME MARCH
enddo
```

```
nrun=nrun+1
write(13,*) nrun
```

```
headlines for output
```

```
111 format(5x,'no. of run=',i3)
112 format(3x,'z(i)',8x,'s(i)',11x,'v(i)',11x,'vnw(i)',10x,'cnw(i)')
113 format(/5x,'time=',f7.3,5x,'z(sat)='f7.2/)
114 format(f8.3,4e15.5)
121 format(5x,'no. of run=',i3,10x,'ibt= ',i3,5x,'iac= ',i3)
122 format(5x,'rn=',f7.3,5x,'qayns=',f6.2,5x,'qaynsc=',f6.2,5x,'qaynwc=',f6.2,5x,'rc=',f6.2/)
123 format(3x,'time',10x,'cnw',11x,'scnw',10x,'scnwc',11x,'sntot',11x,'sccw')
124 format(f8.2,5e15.5)
131 format(5x,'no. of run=',i3,5x,'ccwint=',f7.2,5x,'rc=',f7.2)
132 format(3x,'z(i)',8x,'s(i)',11x,'v(i)',11x,'ccw(i)')
133 format(/5x,'time=',f7.3,5x,'z(sat)='f7.2/)
134 format(f8.3,3e15.5)
```

```
end
```

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PSI(S) FOR UNSATURATED FLOW

```
function psis(s)
common/com1/ssat,smin
common/com12/maspsik
common/com2/alfa,beta,gamma,qaysat
common/psi20/psi0,s1
```

```
maspsik= functions used to clculate psi(s), k(s).
goto (10,20) maspsik
```

10 continue

```
smin= minimal saturation.
psil= suction at s=smin (m).
psir= suction at s=1-epsilon (m).
data psil,psir/0.9,0.7/
psis=psir*(s-smin)/(1.-smin)+psil*(1.-s)/(1.-smin)
goto 100
```

20 continue

```
curve fitting for result from calculations with vG equations.
psis=-psi0*log((s-s1)/(1.-s1))
goto 100
```

100 return

end

QAY(S) FOR UNSATURATED FLOW.

```
function qays(s)
common/com1/ssat,smin
common/com12/maspsik
common/com2/alfa,beta,gamma,qaysat
```

```
goto (10,20) maspsik
```

10 continue

```
qay1,qay2= parameters in K(S) eqution, k=k1(s-smin)+k2(s-smin)**2.
data qay1,qay2/465.5,344.1/
qays=qay1*(s-smin)+qay2*(s-smin)**2
go to 100
```

20 continue

```
Genuchten equation
k=(1-(1-(seq)**(1/gamma))gamma)**2*sqrt(seq)
where:
seq=(s-smin)(ssat-smin)
```

```
seq=(s-smin)/(1.-smin)
seq=min(seq,1.)
qay=(1-(1-(seq)**(1./gamma))**gamma)**2*sqrt(seq)
qays=qay*qaysat
go to 100
```

100 return

end

fort.11

```
&in
teta=.33,ro=2260.,qaysat=2.,alfa=.016,beta=1.3,psi0=66.5,s1=0.4,
smin=.041,ssat=.99,rc=1.,
qayd=4.e3,ckdns=1.,ckdnsc=0.,ckdnwc=0.,cnwm=2.4,elamda=0.,alfan=1.e-4,
ddn=.038,dpor=1.e-4,apec=.63,bpec=1.,
sint=.7,ccwint=1.e5,cnwint=0.,ccwout=1.e5,
hc=100.,dz=1.,dt=0.01,tmax=3001.,tpr=300.,dtpr=30.,maspsik=2,massb=2,
hub=.001,t1=10000.,epss=1.e-6,epsnw=1.e-6,epsnw=1.e-6,
ccwaq=1.e5,cnwaq=0.,ibt=25,iac=26,
consaq=.1,t21=0.,t22=.2,t23=1.0,virrig=0.05
/
CHnwv_Am
```

To Page No. _____

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Invented by _____

Date _____

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This scientific notebook records experimental work conducted to evaluate the importance of rationally being transported in colloidal form. The test code described here was not developed for use in preparing regulatory products. Algorithms tested in the code may be incorporated, at a later date, into the TTA code.

This notebook appears to be well properly maintained.

Arden Wittmeyer
2/8/2000

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I have re-reviewed this scientific notebook and find it in compliance with QAP-001. There is enough information used for conducting tests and developing software so that another qualified individual could repeat the work described herein.

Arden Wittmeyer
2/15/2000

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