Variable definitions and I/O specifications for poulit ver 3.0

Common Types

The common statements are divided into three types and four subtypes. All of the commons labeled /pr*/ contain variables or arrays providing soil profile information. The index of the arrays runs from 0 to izm, with 0 generally referring to the soil surface, and the index referring to positive depth below the surface. Most array variables are functions of time and depth, where depth is $z(i) = i*dz - dz/2$, $z(0) = 0$, and dz is the finite difference space step (cm). "Grid cell centers" refers to the position $z(i)$, while "grid cell boundaries" refers to the position $z(i) + dz/2$. Unless otherwise stated, the index, i, refers to grid cell centers.

All of the common statements labeled /ts*/ contain variables or arrays providing time series information generally related to weather processes. The index of the arrays runs from 0 to iwm, with 1 generally referring to the first day of simulation time, and the index referring to days from start of either simulation or the last application of the litter. The remaining common statement labeled /lo1/ contains logical flags to help with model processing decisions.

Of the subtypes, the common statements labeled /**1/ are double precision real arrays, /**2/ are double precision real scalar variables, /**3/ are integer arrays, and /**4/ are integer scalar variables. Thus, the common statement labeled /pr2/ contains real scalar variables. All real scalars and arrays are double precision whether in common blocks or not.

Note - Many of the dimensions which show as (cm/x) are really $(cm^3/(x\text{-}cm^2))$, a

Soil Profile Info.	Time Series Info.	Logical Flags
Real Arrays /pr1/	Real Arrays /ts1/	/lo1/
Real Scalars /pr2/	Real Scalars /ts2/	
Int. Arrays /pr3/	Int. Arrays /ts3/	
Int. Scalars /pr4/	Int. Scalars /ts4/	

volumetric measurement per square area of land surface.

Common Array And Variable Definitions

common /pr1/

aa(i), bb(i), cc(i) - dummy coefficient arrays for left-hand-side of tridiagonal solution method for diffusive finite difference equations:

$$aa_i x_{i-1} + bb_i x_i + cc_i x_{i+1} = r_i$$

ch(i) - water capacity function, $\partial\theta/\partial h$ (1/cm) at grid cell centers, z(i).

ck(i) - partially saturated soil hydraulic conductivities (cm/h) at grid cell centers.

cv(i) - interblock hydraulic conductivity means (cm/h) at grid cell boundaries, z(i) + dz/2.

ht(i) - total hydraulic head (cm), p(i)-z(i), at cell centers.

p(i) - soil water pressure head (cm) at cell centers.

qme(i) - Imax (ug/(h-cm)) maximum rate of plant nitrogen uptake per unit root length in the Michaelis-Menten approach.

r(i) - dummy array for right-hand-side of tri-diagonal solution for diffusive finite difference methods.

rdist(i) - distribution of root length (cm/cm^3) .

rkd(i) - composite Freundlich adsorption coefficient, $\rho \cdot Kd$ (g/cm^3)$\cdot$(cm^3/g), for NH_4^+.

rx(i) - root extraction rate of water (1/h), (cm^3/(cm^3-h)).

t(i) - soil temperature (°C).

tdif(i) - soil heat diffusion coefficient (cm^2/h).

th(i) - volumetric water content (cm^3/cm^3)

thj(i) - th(i) solved at lst time step

thrr(i) - residual soil water content (cm^3/cm^3)

udl(i) - upper drainage limit (cm^3/cm^3) , the water content at p(i) = -0.1 bar

v(i) - unsaturated water flux (cm^3/(cm^2-h)) at grid cell boundary.

y(i) - NO_3^- concentration in soil solution (ug/ml)

z(i) - depth from soil surface (cm) positive downwards at finite difference grid cell centers, z(i) = (i*dz - dz/2), z(0) = 0.

common /pr2/

ac1, ac2, ac3 - linear coefficients (cm/h) in the unsaturated conductivity relation for soil layers 1, 2, & 3.

at1, at2, at3 - pressure head coefficient (cm) in the soil saturation relation for soil layers 1, ,2 & 3.

bc1, bc2, bc3 - exponential coefficients in the unsaturated conductivity relation of soil layers 1, 2, &3.

bt1, bt2, bt3 - exponential coefficient in soil saturation relation, assumed = 1 in this version.

cev - cumulative actual surface evaporation (cm/h).

cev1 - cev of the previous day.

cl - length of soil column (cm) from the surface to the bottom of soil layer 3.

cl1 - the bottom of soil layer 1 (cm).

cl2 - the bottom of soil layer 2 (cm).

cn - SCS curve number.

disp - solute dispersion coefficient (cm^2/h).

dt - finite difference method time step size (h).

dzl - distance from the bottom of soil layer 3 to the water table (cm).

dz - finite difference method space step size (cm).

dzp - depth increment (cm) for writing soil profile data to file *1.out.

evs - actual surface evaporation (cm/h) limited by soil surface conductivity.

fcu - flux of ammonium (ug/(cm^2-h)) at the soil suface (due to infiltration of litter ammonium).

pl - soil water pressure head (cm) at depth zl (pl = 0 at water table).

pmax - upper limit of soil water pressure head (cm) allowed by model.

qk - Michaelis constant for root nitrogen uptake (ug/ml).

ql - water flux density (cm/h) from bottom of layer 3 to water table.

qm - maximum rate of nitrogen uptake per root length (ug/(cm-h)) in the Michaelis-Menten approach without temperature adjustment.

qu - water flux density (cm^3/(cm^2-h)) or (cm/h) at soil surface due to evaporation and infiltration.

rdnit1, rdnit2, rdnit3 - denitrification rate coefficient, k_2 (1/h) for soils layers 1, 2 & 3.

rex1, rex2, rex3 - ammonium distribution coefficients, Kd (cm^3/g), for soil layers 1, 2 & 3.

rnit1, rnit2, rnit3 - nitrification ratio, k_1 (1/h), for soil layers 1, 2 & 3.

rou1, rou2, rou3 - bulk density, ρ (g/cm^3), of soil layers 1, 2 & 3.

sev - potential soil surface evaporation (cm/h).

thr - residual saturation (cm^3/cm^3) common to all soil layers.

ths1, ths2, ths3 - maximum saturation or porosity (cm^3/cm^3) for soils layers 1, 2 & 3.

tnfin - total nitrogen in the soil column (ug/cm^2) to depth cl at the end of the current day.

wfin - equivalent depth of water (cm) in the soil column to depth cl at the end of the current day.

wilt - plant wilting point soil water pressure head (cm), used to limit root water extraction.

winit - equivalent depth of water (cm) between the surface and the bottom of layer 3 at the start of day.

wk1 - up-gravity weight (0.5 to 1.0) used to create vertical interblock mean hydraulic conductivities from grid cell center conductivities.

wk2 - down-gravity weight, (1-wk1).

zl - depth (cm) to a supposed water table or other constant head boundary.

common /pr4/

l1 - depth index such that z(l1) = cl1.

l2 - depth index such that z(l2) = cl2.

n - depth index such that z(n) = cl.

nm1 - (n-1).

np1 - (n+1).

common /ts1/

crain(n) - cumulative rain (cm) since start of model or nth application of litter.

crdaly(k) - daily rain (0.001 in) from the input weather file *weather.dat.*

csno3(k) - concentration of NO_3^- (ug/ml) in rain infiltration (zero in this version).

et(k) - rate of potential evapotranspiration (cm/h) apportioned to plant transpiration.

fam(n) - fraction of the total nitrogen in the nth litter application mineralized to NH_4^+.

fav(n) - fraction of the total nitrogen in the nth litter application lost to NH_3 volatilization.

fion(n) - fraction of the total nitrogen in the nth litter application apportioned to inorganic nitrogen.

pet(k) - total potential evapotranspiration (cm/h).

runof(k) - rainfall runoff (cm).

tappn(n) - total nitrogen (ug/cm^2) in the nth litter application.

tempmn(k) - daily minimum air temperature (°C).

tempmx(k) - daily maximum air temperature (°C).

xinfl(k) - depth of rain (cm) apportioned to surface infiltration.

common /ts2/

accevp - cumulative total evaporation (cm) (not used in this version).

accpln - cumulative total nitrogen (ug/cm^2) absorbed by plants.

ampd - amount of NH_4^+ in the litter (ug/cm^2) generated per day by mineralization.

aplr - application rate (tons/acre) of litter to land in nth application.

avpd - amount of volatile ammonia (ug/cm^2) generated per day.

cam - total supply of mineralized ammonium in the litter (ug/cm^2) available for rainwater leaching.

caml - cam for the previous day.

csin - total mass of inorganic nitrogen (ug/cm^2) remaining in all n applications of litter.

csinl - csin of the previous day.

csln - NH_4^+ (ug/cm^2) leached from the litter to the soil in one rain.

cslr - total nitrogen remaining undecomposed in the litter (ug/cm^2).

csom - cumulative total nitrogen (ug/cm^2) released by the litter to soil organic matter on completion of mineralization.

cson - total mass of organic nitrogen (ug/cm^2) remaining in all n applications of litter.

csonl - cson of the previous day.

dfam - the fraction of the total nitrogen mineralized to NH_4^+ in the nth litter application in one time step.

dfav - the fraction of the total nitrogen converted to volatile ammonia in the nth litter application in one time step.

dnitr1 - dnitrf of the previous day.

dnitrf - cumulative denitrification (ug/cm^2) of NO_3^- over time.

fci - the fraction of the nth litter application total nitrogen apportioned to inorganic nitrogen.

gwn - total nitrogen released to the groundwater (ug/cm^2) at the end of the day.

gwn1 - gwn of the previous day.

gwnh4 - cumulative mass of NH_4^+ (ug/cm^2) passing from the soil column to the ground water.

gwno3 - cumulative mass of NO_3^- (ug/cm^2) passing from the soil column to the ground water.

gww1 - cumulative volume of water (cm^3/cm^2) passing from the soil column to the ground water by the end of the current day.

gww2 - gww1 for the previous day.

percen - percent of the total litter application mass apportioned to all types of nitrogen.

pln - total nitrogen (ug/cm^2) absorbed by plants in one day.

pln1 - pln for the previous day.

plnh4 - cumulative mass of NH_4^+ (ug/cm^2) absorbed by plants from the soil column.

plnh41 - plnh4 of the previous day.

plno3 - cumulative mass of NO_3^- (ug/cm^2) absorbed by plants from the soil column.

plno31 - plno3 of the previous day.

plnw - cumulative depth of water (cm^3/cm^2) absorbed by plants from the soil column.

plnw1 - plnw of the previous day.

rad - ?

sflux - instantaneous value of water infiltration flux (cm^3/(cm^2-h))

tave - daily average temperature (°C).

tavek - daily average temperature (°K).

time - simulated time (h) since the start of the model.

tinf - time since midnight (h) over which the program spreads the daily rain.

tmax - daily maximum temperature (°C).

tmaxf - daily maximum temperature (°F).

tmin - daily minimum temperature (°C).

tminf - daily minimum temperature (°F).

tninit - total nitrogen (ug/cm^2) in the soil column to depth cl.

twrite - simulation time (h) of the next scheduled output to data files.

xkt - ?

xno3 - total NO_3^- in the soil solution to depth cl (ug/cm^2) .

xtnh4 - total NH_4^+ in the soil column (ug/cm^2) to depth cl.

common /ts3/

kdoy(k) - day of year for kth input from input file *weather.dat*

kyer(k) - (year number - 1900) for the kth input from *weather.dat*

common /ts4/

idd - day of month of weather data input.

imm - month of year of weather data input.

iyr - scalar for kyer(klm).

kday - day of year of the litter application.

klm - number of simulation days since the start of the model or last litter application.

kyr - (year - 1900) of the litter application..

napp - total number of litter applications to date.

nday - scalar for kdoy(klm).

common /lo1/

rday - rain day flag, .true. if rain is currently infiltrating the soil.

vd(i) - soil water flux direction flag, .true. if the direction of the water flux, v(i), is downwards (z-positive) in the soil column at depth $z(i) + dz/2$.

Input Files

unit# file

32   control.dat

15   soils.dat

16   sinit.dat

20   weather.dat

77   appinfo.dat

Input File Descriptions

control.dat

In this program version, this file has one line only, the variable outfs(1), 7 alphanumeric characters, right justified, to concatenate with the output file suffixes, 1.out, 2.out, et cetera, to form the output file names. If the model is to be used repeatedly, a date-based name, such as oc1196a, will be useful for clear record keeping (i.e., oc1196a1.out, etc.).

example:

`oc1196a`

soils.dat

     This file contains soil hydraulic and chemical property information for the three soil layers allowed by the model, as well as other miscellaneous information that the program needs to run. The input format is FORTRAN *-unformated. The program will read space- or comma-delineated ASCII numerical information until its needs are filled. The reader will please refer to the definitions of variables already supplied for common blocks, if not supplied here.

line	input
1	dtt, dzz, dzp - user-supplied time step (h), space step (cm), and profile output step (cm)
2	qm, qk, disp
3	cl, cl1, cl2
4	zl, pl, wk1
5	ac1, bc1, at1, bt1
6	ac2, bc2, at2, bt2
7	ac3, bc3, at3, bt3
8	rou1, ths1, rou2, ths2, rou3, ths3
9	rex1, rnit1, rdnit1
10	rex2, rnit2, rdnit2
11	rex3, rnit3, rdnit3
12	tinf, twrite

example:

```
0.12d0 2.0d0 5.0d0
0.001d0 1.0d0 2.5d0
120.d0 15.d0 45.d0
5000.0d0 0.0d0 0.7071d0
0.1165D-4 0.2500D+2 0.1404D+03 0.1000D+01
0.9560D-6 0.3047D+2 0.2006D+03 0.1000D+01
0.9560D-6 0.3047D+2 0.3004D+03 0.1000D+01
1.28000d0 0.51700d0
1.38000d0 0.47900d0
1.50000d0 0.43400d0
0.15d0 0.02d0 0.01d0
0.15d0 0.001d0 0.01d0
0.25d0 0.001d0 0.01d0
10.d0 24.d0
```

sinit.dat

This file contains necessary initial soil profile data for soil water pressure head, ammonium concentration, nitrate concentration and soil temperature. The data need not match the model finite difference space grid, since it will be linearly interpolated to that grid. Nor do the data for separate variables have to match each other in depth, since they are interpolated from their own depth independent grids. The data can be taken by different means at different depth spacings for each variable.

The first seven lines are dummy or descriptive text comments. Each of the four data variables needs at least three lines of input. The first line contains the integer number of the number of (z,y) data points, nin. The next line contains the z depth ordinates. If that satisfies the nin requirement, the last line contains the y initial variable values. Since the input format is FORTRAN *-unformatted, the program will keep reading lines as necessary until the data requirement is filled.

If one assumes that the data are sparse enough to fit on one line each, the remaining lines would be as follows.

line   data

1   n_{in} - number of data points, (z,p) in the profile

2        $p_1, p_2, ... p_{nin}$ - initial soil water pressure heads (cm)

3        $z_1, z_2, ... z_{nin}$ - at depths z_i (cm) below the soil surface

4   nin - number of points (z,c) in the profile

6        $z_1, z_2, ... z_{nin}$ - at depths z_i (cm)

7   nin - number of data points, (z,y) in the profile

8        $y_1, y_2, ... y_{nin}$ - initial nitrate concentrations (ug/ml)

9        $z_1, z_2, ... z_{nin}$ - at depths z_i (cm)

10   nin - number of data points, (z,T) in the profile

11        $T_1, T_2, ... T_{nin}$ - initial soil temperatures (°C)

12        $z_1, z_2, ... z_{nin}$ - at depths z_i (cm)

example:

```
Each set of data consists of three lines. 1st line
is number of soil measurements, 2nd line is soil depth
and third line is the associated soil data.
The soil data in each of the 3rd lines are initial
values in this order: pressure heads,
NH4-N concentration, NO3-N concentration, and
soil temperature.

7
7 22 37 52 67 82 120
-5000 -2000 -1000 -750 -500 -350 -280
7
7 22 37 52 67 82 120
3.6 0.9 0.3 0.0 0.0 2.2 2.0
```

```
7
7 22 37 52 67 82 120
0.8 0.0 0.0 0.0 0.0 .2 .2
7
7 22 37 52 67 82 120
28.6 25 20 19 18 18 18
```

weather.dat

This input file contains the date, air temperature, and daily rain information. The input data must be contiguous and consecutive from start to end date. The program will stop when it exhausts this file. The reader should refer to the common variable definitions already supplied. FORTRAN i/o format standards are applied. Each line contains the variables:

kyer(klm), kdoy(klm), tempmx(klm), tempmn(klm), crdaly(klm)

in the FORTRAN format (i2, i3, f3.0, f3.0, f5.0). Note that the input value of crdaly is in thousanths of an inch. So, 2000 means 2.000 inches. Directly after input, the program converts the value to centimeters.

example:

```
90 88 51 43    0
90 89 58 49 2000
90 90 56 47  100
90 91 64 46   25
90 92 76 41    0
90 93 59 31    0
90 94 62 38    0
90 95 77 46    0
90 96 63 37    0
90 97 51 28    0
90 98 61 35    0
90 99 62 52    0
90100 66 54    0
90101 55 35    0
90102 49 35    0
90103 62 40    0
90104 62 43    0
90105 69 46 1000
90106 69 46    0
90107 78 40    0
```

appinfo.dat

This file contains the Soil Conservation Service (SCS) curve number for rain runoff in the first line, followed by lines describing the application of poultry litter, if any. The reader should refer to the common variable definitions already supplied. The program will read space- or comma-delineated ASCII numerical information until its needs are filled.

line   variable(s)

1   cn - the SCS curve number for rainfall runoff.

2   kyr, kday, aplr, percen, fci (1st application)

3   kyr, kday, aplr, percen, fci (2nd application)

...

n   kyr, kday, aplr, percen, fci (nth application)

example:

```
  71
 90  88  4  3.79 0.15
 90 100  4  3.79 0.15
```

Output Files

unit#	file
12	*1.out
14	*2.out
25	*3.out
18	*4.out
07	*5.out

Output File Descriptions

File outfs(1)//1.out - water, nitrogen and temperature soil profile data

This output file contains profile data for water, nitrogen and temperature in the soil profile. The first part is essentially a header that reflects the data from the *soils.dat* input file, including explanatory descriptions. The second part consists of three similar sections that repeat every day with rain. The first section gives profile and summary data at the very beginning of the rain day, showing how the soil water, temperature and nitrogen have redistributed since the last rain. The second section gives the same information for the end of the rain infiltration period (ten hours past midnight in this version). Because there is significant redistribution of soil water from the end ot the rain to the end of the day, the third section gives the same information at the end of the day.

Each section has two subsections, profile and summary data. The profile data reports at increasing depth from the soil surface to the bottom of soil layer 3 ($z = cl$) in the nearest finite difference grid steps to intervals of dzp (cm). Each line contains the variables:

$z(i)$, $p(i)$, $th(i)$, $v(i)*24$, $c(i)$, $y(i)$, $t(i)$, $ck(i)*24$

in the FORTRAN format:

(f6.1, 2x, f10.2, 5x, f8.4, 5x, f8.4, 5x, f8.3, 5x, f8.3, 2x, f5.1, 3f8.5)

where the variables are as defined in the section on common blocks.

In this version $v(0)$ is taken to be the same as the upper boundary condition, a combination of evaporation and infiltration. The second subsection displays summary data for :

xno3, xnh4, enh4, xtnh4, xno3+xtnh4, dnit, Δplno3, Δplnh4 & gwn, where

enh4 = total NH_4^+ in the soil exchangeable phase (ug/cm^2) ,

dnit = total nitrogen denitrified (ug/cm^2) for the day,

Δplno3 = plant uptake of NO_3^- (ug/cm^2) for the day,

Δplnh4 = plant uptake of NH_4^+ (ug/cm^2) for the day, and

the other variables are as earlier defined.

File outfs(1)//2.out - soil nitrogen mass balance data

Each line after the header shows the following variables:

klm, iyr, imm, idd, nday, tninit/10, tnfin/10, csln/10, pln/10, accpln/10, dnit/10, gwn/10, tnbal/10, avpd/10, cslr/10

in FORTRAN format (1x, i4, 3i3, i4, 7f9.3, g13.3, 2f9.3), where

tnbal = (tninit - tnfin + csln - pln - dnit - gwn), and

the remaining variables are as defined earlier. Note that dividing the variables by 10 converts from (ug/cm^2) to (kg/ha).

File outfs(1)//3.out - soil water mass balance data

Each line after the header shows the following variables:

klm, iyr, imm, idd, nday, winit, wfin, crdaly(klm), xinfl(klm), dev, runof(klm), gwater, plnup, pet(klm), wbal

in FORTRAN format (1x, i2, 2i3, i4, 9f9.3, g13.3), where

dev = total soil surface evaporation (cm) during one day,

gwater = amount of water (cm) passing from the bottom of soil layer 3 to the ground water since the start of day,

plnup = amount of water (cm) taken up by plants during one day,

wbal = (winit - wfin + crdaly(klm) - runof(klm) - dev - plnup - gwater), the imbalance in soil profile water volume during one day, and the remaining variables are as defined earlier.

Note the dimension of (cm) is actually cm^3 of soil water volume per cm^2 of land surface (cm^3/cm^2).

File outfs(1)//4.out - volatilization, mineralization summary

Each line after the header shows the variables:

iyr, nday, napp, csinl/10, csin/10, avpd/10, csonl/10, cson/10, ampd/10, cam/10, csln/10, cson/10, tave

in FORTRAN format (i2, 2i4, 10f9.3),

where all the variables are as defined earlier. Note that dividing (ug/cm^2) converts to (kg/ha).

File outfs(1)//5.out - nutrient release to ground water

Each line after the header shows the following variables:

iyr, nday, (xno3+xnh4), c(n), y(n), gwn

in FORTRAN format (i4, i5, 4f12.3), where

c(n) = the concentration of NH_4^+ (ug/ml) at the bottom of soil layer 3,

y(n) = the concentration of NO_3^- (ug/ml) at the bottom of soil layer 3, and the remaining variables are as defined before.

Subroutine Parameters

subroutine idist2 (sval)

sval - output, array of 1 ... n, the values of the soil profile variables are linearly interpolated from sparse input file data (*sinit.dat*) to the finite difference method grid positions, z_i, i = 1 to n.

subroutine nextapp (allok)

allok - output, logical flag, set to .false. if the next litter application date from the input file precedes the current simulation date, but does not change from year 1999 to 2000.

subroutine output (eod, ifc)

eod - input, logical flag, set to .true. if *subroutine output* has been called at the end of the simulation day; .false. suppresses output to files *2.out, *3.out, *4.out and *5.out to avoid filling them with partially-calculated data.

ifc - input, integer, the number of times *subroutine compute* has been called in the current simulation day.

subroutine compute (ifc)

ifc - output, integer, the number of times *compute* has been called in the current simulation day, or, the number of time steps, dt, calculated in the simulation day.

subroutine qsf (dz, y, zint, n)

dz - input, size of integration step (usually cm)

y - input, variable of integration over z

zint - output, summation integral of y over z

n - input, integer, number of values of y_i, i = 1, n, to be integrated

subroutine readit (allok)

allok - output, logical flag, set .false. if weather.dat file is exhausted

subroutine tridia (nn, a, b, c, d)

nn - input, length of a, b, c and d arrays (1 ... n)

a, b, c - input, arrays on left hand side of tridiagonal system equation; $a_i * x_{i-1} + b_i * x_i + c_i * x_{i+1} = d_i$, solving for x_i.

d - input, array, right-hand-side of tridiagonal system of equations

d - output, array, x_i solutions to system of equations

subroutine weather (allok)

allok - output, logical flag, .true. if weather.dat file is not exhausted

subroutine wpset (ll, lu, tths, tat, tac, tbc)

ll - input, integer, lowest depth position index of profile properties to be calculated

lu - input, integer, upper depth position index (farther from soil surface) to be calculated

tths - input, value of ths1, ths2, or ths3 being used to calculate soil properties

tat - input, value of at1, at2 or at3 being used

tac - input, value of ac1, ac2 or ac3 being used

tbc - input, value of bc1, bc2 or bc3 being used

function zz1 (m, p, ts)

m - input, integer, soil profile depth index (number of finite difference grid position being used

p - input, soil water pressure head (cm) at depth z(m)

ts - input, soil temperature (°C) at depth z(m)

function zz2 (m, wc, ts)

m - input, integer, soil profile depth index (number of finite difference grid position being used

wc - input, soil water content (cm^3/cm^3) at depth z(m)

ts - input, soil temperature (°C) at depth z(m)