# User's Notes for SPLaSHWaTr

## (**S**imulation **P**rogram for **La**nd-**S**urface **H**eat and **Wa**ter **Tr**ansport)

# Version 2.3

28 June 1991

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# 1. Introduction

These notes describe the input to SPLaSHWaTr, a finite-element program for the solution of the coupled one-dimensional partial differential equations describing heat and water flow in porous media whose pore spaces are filled with water and air, the latter assumed static at constant pressure. These notes describe the assembly and definitions of the input information, and show example input/output for selected problems.

SPLaSHWaTr is a research tool. It is neither user-friendly by current standards, nor is it an expert system. Similarly, this document is not a user's manual, but simply a description of the input. A good degree of modeling expertise is assumed on the part of the user. Some suggestions are offered on the execution of numerical sensitivity analyses, but basically it is asumed that the user will design appropriate numerical experiments, with due attention to principles of numerical simulation.

In its current form, the code is rather inflexible in its specification of soil-dependent physical properties. Generally it is recommended that the user not try to get around this by code modifications since the source code, in its current form, has minimal modularity. Suggested changes or enhancements can be discussed with me.

Units are cgs (centimeter-gram-second), but energy is expressed in calories. Temperature is always in degrees Celsius.

Theoretical background, further documentation of the code, and examples of its application were provided by Milly and Eagleson (1980, 1982) and by Milly (1982, 1984, 1985). Milly and Eagleson (1980) and Milly (1982) described the original development of the code in detail and provided the solutions to sample problems. Milly (1985) described the special numerical technique adopted to conserve mass. Milly and Eagleson (1982) and Milly (1984) modified the code to accept atmospheric forcing as surface boundary conditions, and employed the code in analyses of soil moisture transport, with particular emphasis on thermal effects. Additional work using the code has been reported by Bach (1989), who employed it in the evaluation of laboratory experiments assessing thermal effects on moisture movement in soil, and by Scanlon (1990), who used it in conjunction with isotopic measurements in a preliminary analysis of liquid and vapor transport in an arid field soil.

## 2. Input Data Format

Input is read from a single ASCII file attached to unit 15. The input file has the following structure:

[Part 1]
[Part 2]
[Part 3]

The records in Part 1 are read by the initialization subroutine INIT. Its length is determined by the number of nodes in the spatial discretization. Part 2 is read by the soil initialization subroutine SOILI. Its length is determined by the number of soil types. One record of Part 3 is read each time the boundary conditions change, so its length is determined by the temporal resolution of the input stream (but not of the computations, which may be conducted with a time step smaller than the duration of the input interval).

In the following three subsections, the contents of these three parts of the input file are described. For each read statement in the code, the input list is given in boldface, immediately followed by definitions or explanations of the elements of the input list.

Except for the first record of input (the title, which is read with an A format), all input is free-format. Therefore it is necessary only to separate sequential elements of input by one or more spaces. There should be at least one record (line) in the input file for each input list, but it is acceptable to split one list into one or more input records. Since the input is free-format, it is necessary to enter values for all elements of the list. If a value of a particular variable is not needed to execute a particular run (*e. g.*, Z0 is not used when NBCP is not set to 3), some value must nevertheless be entered for that variable in the input file. In such cases, any value may be entered.

*a. Part 1.*

**(TITLE(I), I=1, 20)**

| | |
|---|---|
| (TITLE(I), I = 1, 20) | Any 80-character sequence used to identify the data set. |

**I1, I2, I3, ... I15**

| | |
|---|---|
| I1 | Set to 1 to obtain printout of initial input data, 0 otherwise. |
| I2 | Set to 1 to obtain printout of the surface boundary condition inputs for each simulation period. |
| I3 | Printout code for water and energy balances. Absolute value follows I4 code. Positive value gives all information, while negative value gives minimal information. |
| I4 | Printout code for moisture content, head, and temperature -<br>0 no printout<br>1 every simulation period<br>2 every time step |
| I5 | Printout code for moisture fluxes. Same code as I4. |
| I6 | Not in use. |
| I7 | Not in use. |
| I8 | Set to 1 for printout of certain parameters in the moisure equation. |
| I9 | Set to 1 for printout of original finite element matrices for moisture. |
| I10 | Set to 1 for printout of algebraic equation for matric head. |
| I11 | Set to 1 for printout of matric head solution from each iteration. |
| I12-I15 | Same as I8-I11, but for heat balance equation and temperature. |

**IFF, IFU, (IF(I), I = 1, 6)**

| | |
|---|---|
| IFF | Unit number to which formatted output (printout) is to be written. |
| IFU | Unit number to which unformatted output is to be written. |
| (IF(I), I = 1, 6) | Parameters specifying frequency with which solution vectors are to be written on IFU. For variable v, IF(v) set to zero allows no writing, and IF(v) set to nonzero k forces writing of vector v at time 0, and after simulation period k, 2k, 3k, etc. Meaning of each v is shown below:<br>1 matric head, PP<br>2 temperature, TT<br>3 absolute humidity of soil air<br>4 moisture content, XX<br>5 water balance components, QWS<br>6 energy balance components, QES |

**NL, NIT, PERR, TERR, XERR**

| | |
|---|---|
| NL | Number of elements into which the soil column is divided. |
| NIT | Number of Picard iterations used during a single time step. |
| PERR | Maximum desirable change in matric head at any node during a single time step. |
| TERR | Maximum desirable change in temperature at any node during a single time step. |
| XERR | Maximum desirable change in moisture content at any node during a single time step. |

**J1, J2, J3, ... J9**

- J1 — Set J1 to 1 to ignore hysteresis, to 0 to allow it.
- J2 — Controls the element-averaging of hydraulic conductivity performed in the subroutine MAT. A value of 1 yields the geometric mean of nodal values, which has been shown to be superior in terms of general accuracy. A value of 0 gives the arithmetic mean, which has the desirable property of being non-zero when only one nodal value is non-zero, thereby allowing infiltration to occur into soil whose initial K is zero. An alternative to the use of J2=0 for this problem is to set CKMIN to some small value (<<CKSAT) greater than zero.
- J3 — Traditional treatment of moisture capacity during time-stepping if equal to 0, with very poor mass balance performance. Much better resuts with a value of 1, which invokes Milly's (1985) method.
- J4 — Set to 0 for no lumping of mass matrix, to 1 and 2 for different lumping schemes. Value of 2 is recommended, since that has been used in most development and application.
- J5 — Same as J4, but for energy matrix.
- J6 — Specifies system of equations to be solved -
  - 0 Full system of Milly (1982)
  - 5 Ignore water vapor, heat of wetting, and temperature effects on hydraulic conductivity and water retention
  - 6 Solve only the Richards equation
- J7 — Not in use.
- J8 — Choice of curve defining main wetting curve at reference temperature -
  - 0 Use the following (Milly and Eagleson, 1982, Eq. 2.21):

$$\theta_w(\psi) = min\left(XU,\ AA\left(\frac{\psi}{BB}\right)^{CC} + DD\,(7 - \log(-\psi)) + EE\right)$$

  - 1 Use the following (Van Genuchten, 1980):

$$\theta_w(\psi) = (XU - AA)\left[1 + (BB\psi)^{CC}\right]^{-DD} + AA$$

  - 2 User definition. Must insert source code in subroutines SOILI and XWET.
- J9 — Choice of method for specifying the relative hydraulic conductivity function -
  - 0 Numerical integration of Mualem's expression.
  - 1 Analytic integration of Mualem's expression, available only for the case when J8=1.
  - 2 User definition. Must insert code in subroutine SOIL3.

**NS, DSTMAX, TZERO, Z0, ZA, CKMIN**

- NS — Number of soil types.
- DSTMAX — Depression storage capacity of soil surface.
- TZERO — Temperature at which input soil parameters apply.
- Z0 — Surface roughness parameter, used only if NBCP=NBCT=3.
- ZA — Height at which meteorological inputs apply, used only if NBCP=NBCT=3.
- CKMIN — Lower limit to be set on hydraulic conductivity. Set to zero to avoid spurious negative values. See also J2.

**NBCPB, NBCTB, BCPB, BCTB**

| | |
|---|---|
| NBCPB | Type of boundary condition on matric head at bottom of column, held fixed for the entire simulation -<br>1 specified head of BCPB at bottom node<br>2 speicifed moisture flux of BCPB at bottom node<br>3 zero matric head gradient at bottom node (gravity drainage) |
| NBCTB | Type of boundary condition on temperature at bottom of column, held fixed for the entire simulation -<br>1 specified temperature BCTB at bottom node<br>2 specified heat flux at BCTB at bottom node<br>3 zero temperature gradient at bottom node (advection only) |
| BCPB | See NBCPB. Not used if NBCPB is 3. |
| BCTB | See NBCTB. Not used if NBCTB is 3. |

**Z(1), P(1), T(1)**

**Z(2), P(2), T(2)**

**...**

**Z(NN), P(NN), T(NN)**

| | |
|---|---|
| Z(I) | For each node I (numbered from the bottom up), this is the elevation (positive upward) |
| P(I) | For each node I, the initial value of matric head |
| T(I) | For each node I, the initial value of temperature |

**IS(1), IH(1), XWRE(1,1), XWRE(1,2)**

**IS(2), IH(2), XWRE(2,1), XWRE(2,2)**

**...**

**IS(NL), IH(NL), XWRE(NL,1), XWRE(NL,2)**

| | |
|---|---|
| IS(L) | For each element L (numbered from the bottom up), this is the index (< or = NS) of the soil type of that element. |
| IH(L) | For each element L, a flag indicating wetting (1) or drying (2) of element |
| XWRE(L,1) | If IH(L) is 1, element L is assumed to be initially wetting after leaving the main drying curve at a value of matric head for which the corresponding main wetting function has value XWRE(L,1) at the bottom node of element L. If IH(L) is 2, element L is drying after leaving the main wetting curve at moisture content XWRE(L,1) at the bottom node. |
| XWRE(L,2) | Same as XWRE(L,1), but for upper node of element L. |

*b. Part 2. Repeat this set of input for J = 1, NS.*

**POR(J), XU(J), CKSAT(J), AA(J), BB(J), CC(J), DD(J), XK(J)**

| | |
|---|---|
| POR(J) | Total volumetric porosity |
| XU(J) | Moisture content upon re-wetting: porosity minus entrapped air |
| CKSAT(J) | Hydraulic conductivity at moisture content XU(J) |
| AA(J) - DD(J) | Parameters defining main wetting curve. See J8 in part 1. For J8 =0, the value of EE consistent with the values given for XU and AA-DD is computed internally in SOILI. For J8=1, the value of DD input is ignored, and DD is re-computed internally using AA-CC and XU. User may employ AA-DD for J8=2, if desired. |
| XK(J) | Highest moisture content at which isothermal liquid flow is small relative to isothermal vapor flow. Used by subroutines SOIL3 and SOIL4, but only when J6 is 0 or 5. |

**(VPER(J,K), K = 1, 3), DUM1, DUM2, DUM3, DUM4, SSUR**

| | |
|---|---|
| VPER(J,1) | Volumetric fraction of soil type J occupied by quartz particles. Not used when J6 is 6. |
| VEPR(J,2) | Volumetric fraction of soil type J occupied by other minerals. Not used when J6 is 6. |
| VPER(J,3) | Volumetric fraction of soil type J occupied by organic matter. Not used when J6 is 6. |
| DUM1 - DUM4 | Significant only for soil type found in the top element. Then DUM1 and DUM2 are the albedoes of dry and wet soil, and DUM3 and DUM4 are the emissivities of dry and wet soil. Used only when NBCP = NBCT =3. |
| SSUR | The specific surface of the soil type for which data is currently being read. Not used when J6 is 5 or 6. Then set it to 1. |

*c. Part 3. Repeat this set of input for as many simulation periods as desired.*

**DURTN, DLT, NBCP, NBCT, A1, A2, A3, A4, A5, A6**

| | |
|---|---|
| DURTN | The duration of this simulation period (period of fixed boundary conditions), in seconds |
| DLT | Initial times step size to begin the simulation period. If negative, the time step size will be determined in the usual way from the results of the previous time step. Ordinarily, a small value (one second or smaller) is advised for starting a simulation. |
| NBCP | Code for type of surface boundary condition on mass equation to be applied during the simulation period -<br>1 specified matric head<br>2 specified potential moisture flux (potential evaporation rate or precipitation rate)<br>3 specified atmospheric forcing<br>If NBCP is set to 3, it must be so for all simulation periods, and then NBCT must also be 3, and *vice versa*. Atmospheric forcing can not be used if J6 is 6. |
| NBCT | Code for type of surface boundary condition on heat equation to be applied during the simulation period (see NBCP above) -<br>1 specified temperature<br>2 specified heat flux<br>3 specified atmospheric forcing |
| A1 - A6 | Significance depends on whether or not NBCP and NBCT are 3. If so, then these are atmospheric forcing variables -<br>A1 precipitation rate<br>A2 absolute humidity of air at height ZA (Part 1)<br>A3 windspeed at height ZA<br>A4 incoming solar radiation<br>A5 incoming longwave radiation<br>A6 temperature of air at height ZA<br>If NBCP and NBCT are not 3, then A3 through A6 are not used. If NBCP is 1, then A1 is the specified head. If NBCP is 2 , then A1 is the potential moisture flux (positive upward).<br>If NBCT is 1, then A2 is the specified temperature. If NBCT is 2, then A2 is the specified heat flux (positive upward). |

## 3. Selection of Iteration and Time Step Parameters

Most of the input variables for SPLaSHWaTr are physical variables or simulation options; their specification is usually straightforward for a well-defined physical problem. Some important exceptions are NIT, PERR, XERR, and TERR, as well as the number and spacing of the nodes. These all relate to the numerical approximation applied in the solution of the governing equations. The accuracy of the solution, and even its attainability, are critically sensitive to these parameters.

At each time step, it is necessary to solve a nonlinear system of equations. SPLaSHWaTr obtains a solution by successively linearizing and solving the equations, with the number of iterations for each time step specified by the user. There is a tradeoff between the time step duration and the number of iterations necessary to achieve convergence of the nonlinear solution, since larger time steps mean larger changes in state, and hence greater departures from linear behavior. Experience has generally shown that it is more efficient to keep the number of iterations small and insead to control accuracy by varying the time step size. However, some amount of iteration is necessary in order to take advantage of the method for evaluation of the moisture capacity, which has been designed to ensure highly accurate balances of mass. The parameter NIT can thus be chosen on the basis of sensitivity analyses and the desired degree of mass balance; a value of 2 to 4 usually suffices. See Milly (1985).

At the end of each time step, PERR, TERR, and XERR are used to determine a new time step size automatically. The step size is maximized subject to the constraint that no change in any nodal value of the states should exceed these prescribed upper limits during the next time step, assuming that the rates of changes of nodal values will be the same as in the previous time step. Thus the new time step size is found as

$$\Delta t = min\left[\frac{\text{PERR}}{max_i\left(\frac{d\psi_i}{dt}\right)}, \frac{\text{TERR}}{max_i\left(\frac{dT_i}{dt}\right)}, \frac{\text{XERR}}{max_i\left(\frac{d\theta_i}{dt}\right)}\right] \qquad (1)$$

where $max_i$ denotes maximization over all nodes i, and the rates of change are estimated from the most recent time step. Since rates of change vary from one step to the next, there is no guarantee that the change of state will not exceed the desired limit PERR, TERR, or XERR; indeed, chances are that it will. If it turns out that any desired change is exceeded by the actual change by a factor greater than four on any given time step, the results of that time step are discarded, and the time step is repeated with a proportionately smaller duration. However, when a finite change in one of the states is forced by the specification of a first-type boundary condition (NBCP or NBCT equal to 1) then that node is not included in (1), since the time step could otherwise go to zero due to the backtracking algorithm described above. If the application of (1) suggests an increase in time step by a factor greater than 6, the increase is limited to a factor of 6. There is a certain amount of redundancy in the combination XERR, TERR, and PERR. Generally one might set PERR equal to $10^7$ cm so that it will not be binding, and instead use XERR to control the time step from a moisture point of view.

The actual magnitudes of PERR, TERR, and XERR prescribed will depend on the problem solved and the objectives of the study. Ideally, one would repeat the same simulation many times over with various values for these parameters, noting the convergence of the solution with increasingly small times steps, and then choose the values of the parameters that gave a reasonable tradeoff between computational effort and solution accuracy. An example of such an analysis was presented by Milly and Eagleson (1982), who also addressed the question of optimal spatial resolution.

## 4. Known Bugs and Possible Future Improvements

There are problems with the convergence of the solution to the nonlinear equation for surface matric head when the soil surface is in the vicinity of saturation. This is particularly troublesome, since the code does not check whether or not the iteration process converges before starting a new time step. The problem seems to be avoided when the soil moisture characteristic has a sharp corner in it at saturation , *e. g.*, when one uses J8 equal to 0 or when a Brooks-Corey form is specified under J8 equal to 2. When the problem occurs, subsequent iterative estimates of surface matric head do not converge to a unique value. If several iterations are allowed, the values will eventaully oscillate between two distinct values, one saturated (or almost so) and the other unsaturated. It appears that the only way to remove this problem for any soil moisture characteristic will be to change the iterative algorithm from the simplistic Picard iteration to a more robust, brute-force method, such as bisection. The switch from one scheme to the other in actual simulations might be determined on the basis of convergence or non-convergence of the iterative process. This code improvement will involve rather substantial code changes, and has not been implemented yet.

Several other future code changes have been identified as being desirable --

- Remove numeric constants from various executable statements and collect in one place as variables.
- Increase the flexibility and modularity in the specification of soil-dependent physical functions, instead of hard-wiring them into the code.
- Provide summary information on time step sizes.
- Set up the program as a subroutine in order to facilitate interfacing with other programs, pre-processors, and post-procesors.
- Incorporate a simple vagetation canopy, allowing for water extraction by roots, interception by foliage, and shading of the ground by foliage.

## 5. Sample Input and Output Files

Printouts of three sample input and output files are appended to these notes. The first two are simple isothermal infiltration problems, and the third uses the full system of equations in conjunction with atmospheric forcing.

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