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1. INTRODUCTION

As part of the work performed to model flow in the unsaturated zone at Yucca Mountain, Nevada, a capillary hysteresis model has been developed. The computer program HYSTR has been developed to compute the hysteretic capillary pressure - liquid saturation relationship through interpolation of tabulated data. The code can be easily incorporated into any numerical unsaturated flow simulator. A complete description of HYSTR, including a brief summary of the previous hysteresis literature, detailed description of the program, and instructions for its incorporation into a numerical simulator are given in the HYSTR user's manual (Niemi and Bodvarsson, 1991a).

This report describes the incorporation of HYSTR into the numerical code TOUGH (Transport of Unsaturated Groundwater and Heat; Pruess, 1986). The changes made and procedures for the use of TOUGH for hysteresis modeling are documented. A full description of TOUGH and its use are given in Pruess (1986). The following chapters are meant to be used only as a supplement for that document.

2. INCORPORATION OF HYSTR INTO TOUGH

The set of subroutines performing the actual hysteresis simulation (calculating the capillary pressure for given liquid saturation and for given wetting/drying history of the element) is called by TOUGH through a main subroutine PCHYST, which replaces the subroutine PCAP for the materials for which hysteresis is considered. Subroutine SAVEHS is used for storing the wetting/drying history information from one time step to the next; this routine is only called when convergence is achieved. The tabulated hysteresis data for each hysteretic material are read from a new data block HYSTR. Additional initial condition information is read in through the block INCON.

To assure the continuity of the derivatives, the hysteresis calculation is designed in such a way that the $\phi = \phi(S_l)$ curve is only chosen once for each Newton-Raphson iteration. This curve is selected only when the calculation is made with the actual primary variables ($k = 1$). When each primary variable is then incremented during the same iteration ($k = 2, 3, 4$) to obtain the derivatives for the Jacobian matrix, the same curve is used. The continuity of the derivatives is necessary to allow rapid convergence of the iteration.

3. CHANGES IN TOUGH INPUT

To use the hysteretic capillary pressure - liquid saturation relationship option with TOUGH, changes have to be made in the data blocks INCON and ROCKS and one new data block (HYSTR) has to be added. The changes are (notation as in Pruess (1986)):

ROCKS:

Card ROCKS.1.2

IRP has to be chosen such that relative permeability will be calculated as a function of liquid saturation rather than capillary pressure for the materials for which ICP is selected as 100 (specified in card ROCKS.1.3). In standard TOUGH, k_{rl} is always computed as a function of S_l, but in some modified versions $k_{rl} = k_{rl}(\phi)$ has also been used. Calculating $k_{rl} = k_{rl}(\phi)$ will not create obvious problems, but will be inconsistent with the reasoning given in Niemi and Bodvarsson (1991b): hysteresis can be ignored in the $k_{rl} = k_{rl}(S_l)$ relationship but not in the $k_{rl} = k_{rl}(\phi)$ relationship if the hysteretic $\phi = \phi(S_l)$ is assumed.

Card ROCKS.1.3

ICP = 100 for the materials for which a hysteretic capillary pressure - liquid saturation relationship is assumed.

Note that hysteretic materials must be listed before the non-hysteretic types in the data block ROCKS.

INCON:

The following data should be read in for all elements (including the ones for which hysteresis is not considered):

Card INCON.1 [Format(a3, i2,2i5,e15.8,i10)]

EL,NE	see Pruess (1986)
NSEQ	"
NADD	"
PORX	"
ICRV	type of the initial curve = 1 when starting from the main drying curve = 2 when starting from the main wetting curve = 3 when starting from a drying scanning curve = 4 when starting from a wetting scanning curve

Card INCON.2 [Format(4e20.13)]

X1	see Pruess (1986)
X2	"
X3	"
PCINI	initial capillary pressure (Pa), as solved from the chosen curve (see ICRV) for the given initial liquid saturation

Card INCON.3 [Format (e20.14,4I5)]

This card specifies the location of the starting point (defined by the initial liquid saturation and PCINI of the element) relative to the adjacent tabulated scanning curves of corresponding type. The values specified in this card are only needed if the starting point is on a scanning curve (ICRV = 3 or 4), otherwise a blank line can be given.

RATI1	= X1/X2, where X1 is the difference in SL between the starting point and the tabulated scanning curve of proper type above it X2 is the difference in SL between the tabulated scanning curves above and below the starting point at pressure PCINI

NN11 — number of the tabulated scanning curve of proper type above the starting point (No. 1 corresponds to the lowest curve)

NN21 — number of the tabulated scanning curve of proper type below the starting point

K11 — number of tabulated values on curve number NN11

K21 — number of tabulated values on curve number NN21

HYSTR:

Card HYSTR.1 [Format(I5,e10.3,2a5)]

LOGR — capillary pressure input parameter

= 1 if capillary pressures in the hysteresis loop are input in a logarithmic scale

= 0 if capillary pressures are input in linear scale

EPSLN — reversal criterion that specifies the minimum difference in liquid saturation between two consecutive time steps that can result in a reversal from the previous curve

ELEHS1, ELEHS2 — element names for two elements for which printouts of capillary pressure and liquid saturation are given after every time step

For each hysteretic material, the following cards HYSTR.2.1...2.4 must be specified to tabulate the hysteresis loops. An example of a tabulated set of hysteresis curves is given in Fig. 1.

The materials need to be in the same order as in the ROCKS data block.

Card HYSTR.2.1 [(Format(a3,a2,3I5)]

A1,A2 — material name; must be the same five letter identifier used in the block ROCKS for the material in question

L1 — number of tabulated sets of values on the main boundary curves

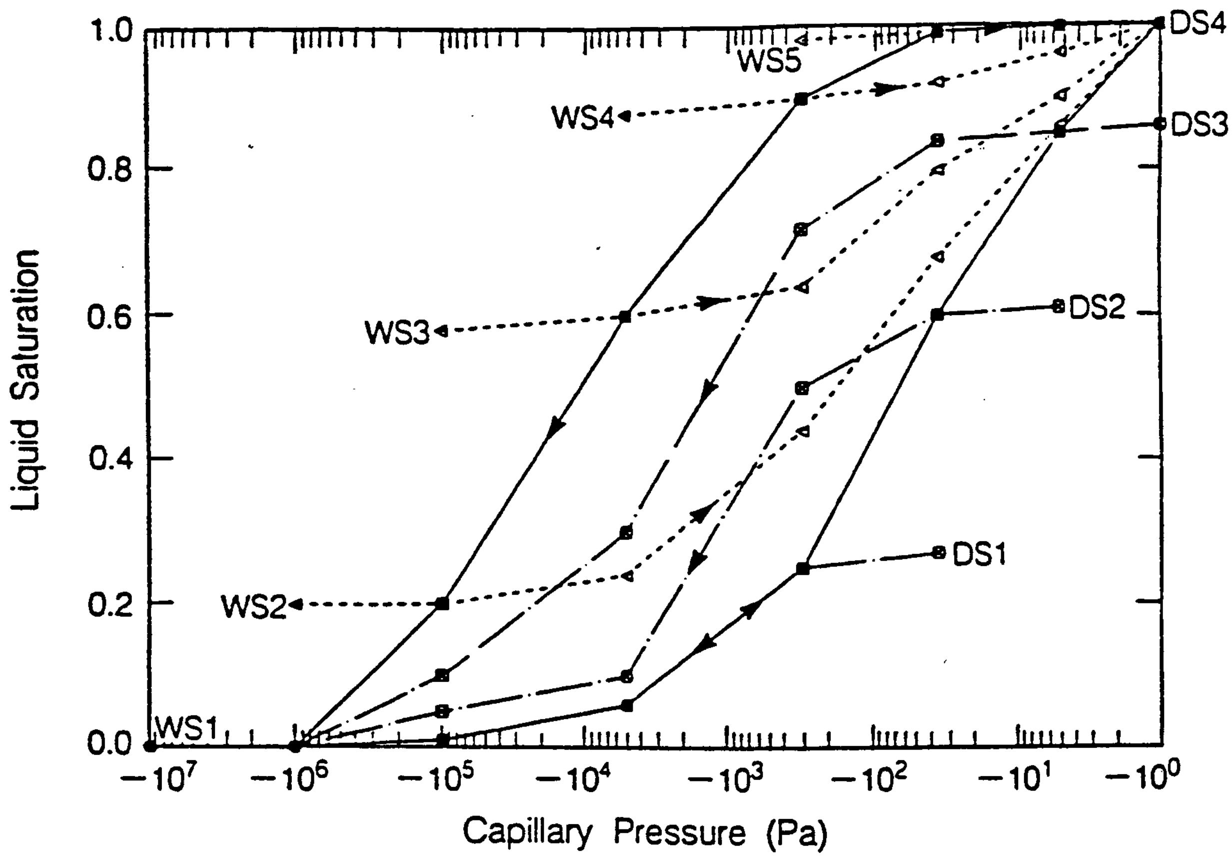

Figure 1. Example of a tabulated hysteresis data. WS1 . . . WS5 are tabulated wetting scanning curves. DS1 . . . DS4 are tabulated drying scanning curves.

L2 number of tabulated drying scanning curves

L3 number of tabulated wetting scanning curves

Card HYSTR.2.2 [Format(10x,3e10.3)]

This card defines the main boundary curves. Input L1 sets of values running from left to right with a hysteresis loop such as those in Fig. 1.

PSIVAR(j,n) capillary pressure value (Pa)

SDRY(j,n) liquid saturation value on the main drying curve corresponding to PSIVAR(j,n)

SDRY(j,n) liquid saturation value on the main wetting curve corresponding to PSIVAR(j,n)

Card HYSTR.2.3

This card defines the primary drying scanning curves. Tabulate for L2 curves starting from the lowest curve (see Fig. 1). Nodes on each curve have to be tabulated from right to left.

Card 2.3.1 [Format(i5)]

K10 number of tabulated values on the drying scanning curve

Card 2.3.2 [Format(10x,2e10.3]

Repeat this card K10 times.

DDP(i,j,n) capillary pressure value (Pa)

DDS(i,j,n) liquid saturation on the tabulated drying scanning curve corresponding to DDP(i,j,n)

Card HYSTR.2.4

This card defines the primary wetting scanning curves. Tabulate for L3 curves starting from the lowest curve. Values on each curve must be tabulated from left to right.

Card 2.4.1 [Format(i5)]

K20 number of nodes on the tabulated wetting scanning curve

Card 2.4.2 [Format(10x,2e10.3)]

Repeat this card K20 times.

WP(i,j,n) capillary pressure value (Pa)

WS(i,j,n) liquid saturation on the tabulated wetting scanning curve corresponding to WP(i,j,n)

Card HYSTR.3 A blank card ends the HYSTR data block

An example input file demonstrating these changes is given in appendix A. The tabulated hysteresis curves in this input file are those shown in Figure 1. Detailed instructions on the tabulation of the curves are given in Niemi and Bodvarsson (1991a).

4. CHANGES IN TOUGH OUTPUT

The following changes have been made in the TOUGH output:

(a) Output on the files SAVE and INCON is changed to be compatible with the modified input in the block INCON. In addition to the normal output capillary pressures, curve types and information on the location at the last turning point are also given in these files. This enables the normal use of continuation runs and the start option.

(b) Data given in data block HYSTR will automatically be printed on the main output file regardless of the value of MOP(7).

5. DIMENSIONING OF THE ARRAYS

Dimensioning of the different arrays in hysteresis routines should be made according to the following tabulation:

```
common/prssat/psivar(nb,nmt),sdry(nb,nmt),swet(nb,nmt)
common/dscan/ddp(nns,ncs,nmt),dds(nns,ncs,nmt)
common/wscan/wp(nns,ncs,nmt),ws(nns,ncs,nmt)
common/tab/ltabps(nmt),ltabd(nmt),ltabw(nmt)
common/tab2/kd(ncs,nmt),kw(ncs,nmt)
common/icon/icurv(ne),pcin(ne)
common/savehr/pold(ne),sold(ne)
common/tmphys/ptmpo(ne),stmpo(ne),ktmpo(ne)
common/calc/k1(ne),k2(ne),ratio(ne),nn10(ne),nn20(ne)
common/savecr/nn1sa(ne),nn2sa(ne),ratisa(ne),icntr(ne),
k1sa(ne),k2sa(ne)
a(nns,ncs,nmt),b(nns,ncs,nmt)
```

where

ne	= number of elements
nmt	= number of materials
nns	= maximum number of tabulated nodes on any scanning curve
ncs	= maximum of the following two values: number of tabulated drying scanning curves or number of tabulated wetting scanning curves
nb	= number of tabulated nodes on main boundary curves

6. APPLICABILITY AND LIMITATIONS

- The main advantage of HYSTR is, that any kind of measured hysteresis data can be easily incorporated and accurately modelled with it in case of wetting and drying along the main boundary as well as along the first order scanning curves.
- The model is based on the assumption that second and higher order scanning curves can be approximated from the tabulated first order scanning curves. With frequent reverses from wetting to drying and vice versa, this assumption produces an erroneous "pumping effect" (see Klute and Heermann (1974), Jaynes (1984), and Niemi and Bodvarsson (1991b) for examples). It has been suggested (Banergee and Watson, 1984) that this kind of approach should not be used when reversals are too closely spaced in time. We recommend that when modeling cyclic wetting/drying pulses use of some other model designed to avoid "pumping," should be considered. Further discussions are presented in for example Niemi and Bodvarsson (1991b), in which we also present two hysteresis models that do not exhibit "pumping."
- When using HYSTR as incorporated in TOUGH the initial time step should be large enough that some changes in the primary variables occur during the first time step. If there are no changes during the first iteration of the first time step the program does not call subroutine EOS during this time step. This in turn causes the hysteresis "history" to be initialized incorrectly.

7. REFERENCES

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APPENDIX A

Sample of the Input Changes

```
this is a sample file to demonstrate the changes in TOUGH input due to HYSTR
ROCKS
HYS1       ******************************************
           ******************************************
   70      (IRP chosen such that K=K(SL)
  100      (ICP)
HYS2       ******************************************
           ******************************************
   70
  100
NOHYS      (non hysteretic materials listed after the hysteretic ones)

   99
   99

START
PARAM
*
*
TIMES
*
*
*
ELEME
E   1            NOHYS 0.500e+00
E   2            HYS1  0.500e+00
E   3            HYS2  0.158e+01

CONNE
*
*
*

GENER
*
*
*

HYSTR
    1       1.e-4E    2E    3  (LOGR,EPSLN,ELEHS1,ELEHS2)
HYS1       7    4    5     (A1,A2,..FOR 1. MATERIAL, SL-PCAP AS IN FIGURE 1.)
            -0.100E+07 0.000E+00 0.000E+00 tabulation of boundary curves
            -0.100E+06 0.200E+00 0.100E-01
            -0.500E+04 0.600E+00 0.600E-01
            -0.300E+03 0.900E+00 0.200E+00
            -0.350E+02 0.990E+00 0.600E+00
            -0.500E+01 0.997E+00 0.850E+00
            -0.100E+01 0.100E+01 0.100E+01
    5                                      lowest drying scanning curve (DS1)
            -0.350E+02 0.270E+00
          - -0.300E+03 0.250E+00
            -0.500E+04 0.600E-01
            -0.100E+06 0.100E-01
            -0.100E+07 0.000E+00
    6                                        (DS2)
            -0.500E+01 0.610E+00
            -0.350E+02 0.600E+00
            -0.300E+03 0.500E+00
            -0.500E+04 0.100E+00
            -0.100E+06 0.500E-01
```

```
        -0.100E+07 0.000E+00
    7                                          (DS3)
        -0.100E+01 0.860E+00
        -0.500E+01 0.850E+00
        -0.350E+02 0.840E+00
        -0.300E+03 0.720E+00
        -0.500E+04 0.300E+00
        -0.100E+06 0.100E+00
        -0.100E+07 0.000E+00
    8                                          uppermost drying scanning curve (DS4)
        -0.500E+00 0.100E+01  --actual value of this imag.node doesnt matter-
        -0.100E+01 0.999E+00
        -0.500E+01 0.997E+00
        -0.350E+02 0.990E+00
        -0.300E+03 0.900E+00
        -0.500E+04 0.600E+00
        -0.100E+06 0.200E+00
        -0.100E+07 0.000E+00
    8                                     lowest tabulated wetting curve (WS1)
        -0.100E+08 0.000E+00  --actual value of this imag.node doesnt matter--
        -0.100E+07 0.100E-02
        -0.100E+06 0.100E-01
        -0.500E+04 0.600E-01
        -0.300E+03 0.250E+00
        -0.350E+02 0.600E+00
        -0.500E+01 0.850E+00
        -0.100E+01 0.100E+01
    7                                     (WS2)
        -0.100E+07 0.199E+00
        -0.100E+06 0.200E+00
        -0.500E+04 0.240E+00
        -0.300E+03 0.440E+00
        -0.350E+02 0.680E+00
        -0.500E+01 0.860E+00
        -0.100E+01 0.100E+01
    6                                     (WS3)
        -0.100E+06 0.580E+00
        -0.500E+04 0.600E+00
        -0.300E+03 0.640E+00
        -0.350E+02 0.800E+00
        -0.500E+01 0.900E+00
        -0.100E+01 0.100E+01
    5                                     (WS4)
        -0.500E+04 0.880E+00
        -0.300E+03 0.900E+00
        -0.350E+02 0.920E+00
        -0.500E+01 0.960E+00
        -0.100E+01 0.100E+01
    4                                     (WS5)
        -0.300E+03 0.989E+00
        -0.350E+02 0.990E+00
        -0.500E+01 0.997E+00
        -0.100E+01 0.100E+01
HYS2     7    4    5 (SL-PCAP AS IN FIG.1 ,WITH  PCAP-VALUES MULTIPLIED BY 100)
        -0.100E+09 0.000E+00 0.000E+00 tabulation of boundary curves
        -0.100E+08 0.200E+00 0.100E-01
        -0.500E+06 0.600E+00 0.600E-01
        -0.300E+05 0.900E+00 0.200E+00
        -0.350E+04 0.990E+00 0.600E+00
        -0.500E+03 0.997E+00 0.850E+00
```

```
     -0.100E+03 0.100E+01 0.100E+01
5                                  lowest drying scanning curve (DS1)
     -0.350E+04 0.270E+00
     -0.300E+05 0.260E+00
     -0.600E+06 0.600E-01
     -0.100E+08 0.100E-01
     -0.100E+09 0.000E+00
6                                   (DS2)
     -0.600E+03 0.610E+00
     -0.350E+04 0.600E+00
     -0.300E+05 0.500E+00
     -0.600E+06 0.100E+00
     -0.100E+08 0.500E-01
     -0.100E+09 0.000E+00
7                                   (DS3)
     -0.100E+03 0.860E+00
     -0.600E+03 0.850E+00
     -0.350E+04 0.840E+00
     -0.300E+05 0.720E+00
     -0.600E+06 0.300E+00
     -0.100E+08 0.100E+00
     -0.100E+09 0.000E+00
8                                   uppermost drying scanning curve (DS4)
     -0.600E+02 0.100E+01  --actual value of this imag.node not important
     -0.100E+03 0.999E+00
     -0.600E+03 0.997E+00
     -0.350E+04 0.990E+00
     -0.300E+05 0.900E+00
     -0.600E+06 0.600E+00
     -0.100E+08 0.200E+00
     -0.100E+09 0.000E+00
8                               lowest tabulated wetting curve (WS1)
     -0.100E+08 0.000E+00  --actual value of this imag.node not important
     -0.100E+09 0.100E-02
     -0.100E+08 0.100E-01
     -0.600E+06 0.600E-01
     -0.300E+05 0.250E+00
     -0.350E+04 0.600E+00
     -0.600E+03 0.850E+00
     -0.100E+03 0.100E+01
7                               (WS2)
     -0.100E+09 0.199E+00
     -0.100E+08 0.200E+00
     -0.600E+06 0.240E+00
     -0.300E+05 0.440E+00
     -0.350E+04 0.680E+00
     -0.600E+03 0.860E+00
     -0.100E+03 0.100E+01
6                               (WS3)
     -0.100E+08 0.580E+00
     -0.600E+06 0.600E+00
     -0.300E+05 0.640E+00
     -0.350E+04 0.800E+00
     -0.600E+03 0.900E+00
     -0.100E+03 0.100E+01
5                               (WS4)
     -0.600E+06 0.880E+00
     -0.300E+05 0.900E+00
     -0.350E+04 0.920E+00
     -0.600E+03 0.960E+00
```

```
          -0.100E+03 0.100E+01
    4                                     (WS5)
          -0.300E+05 0.989E+00
          -0.350E+04 0.990E+00
          -0.500E+03 0.997E+00
          -0.100E+03 0.100E+01

INCON
E   1           0.50000001E-01          0
 1.0000000000000E+06 0.9999489554516E+00 0.2600000865167E+02-0.1359000000000E+07

E   2           0.13880000E+00          1
 1.0000000000000E+06 0.6000000000000E+00 0.2600000865461E+02-2.0000000000000E+04

E   3           0.13880000E+00          4
 1.0000000000000E+06 0.6000000000000E+00 0.2600000866931E+02-1.0000000000000E+06
 0.78571430000000000      3    2    6    7

ENDCY
```

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