Scientific Notebook No. 184: Thermal Effects on Flow Key Technical Issue--Investigation of the Effects of Repository Heating on Perched-Water Evolution of Yucca Mountain (03/20/1996 through 07/15/1999)

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Goodluck OFOEGBU

CNWRA

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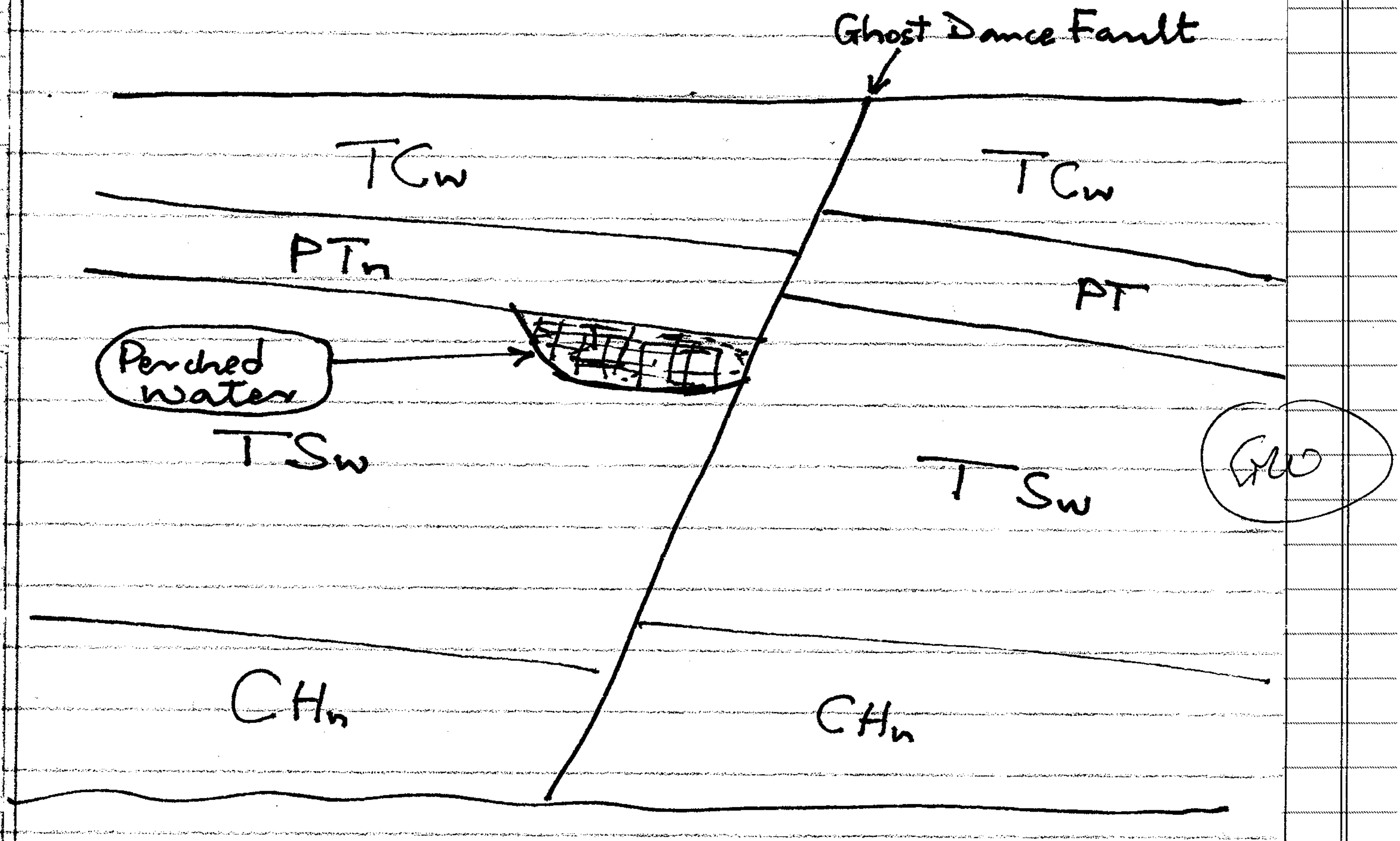
Initial Entry: March 20 1996

GW

Thermal Effects on Flow KTI
Investigation of the Effects of Repository Heating on Perched-Water Evolution at Yucca Mountain (YM).

Investigations conducted under Isothermal Flow KTI demonstrate stratigraphic and structural-geologic controls on perched-water formation at YM.



In the current project simulated repository heating will be applied to a moisture distribution calculated under isothermal conditions. The evolution of perched water ~~will be monitored~~ following the introduction of heating will be monitored for the short time

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(tens of years), intermediate time (hundreds of years), and long time (thousands of years).

Analyses will be conducted using METRA (the nonisothermal-flow module of MULTIFLO). See the METRA 1.0 Users' Manual (CNWRA 96-005) for more information about METRA and MULTIFLO.

Investigators: Goodluck I Ofoegbu
Amvrossios C Bagtzoglou
Michael Muller

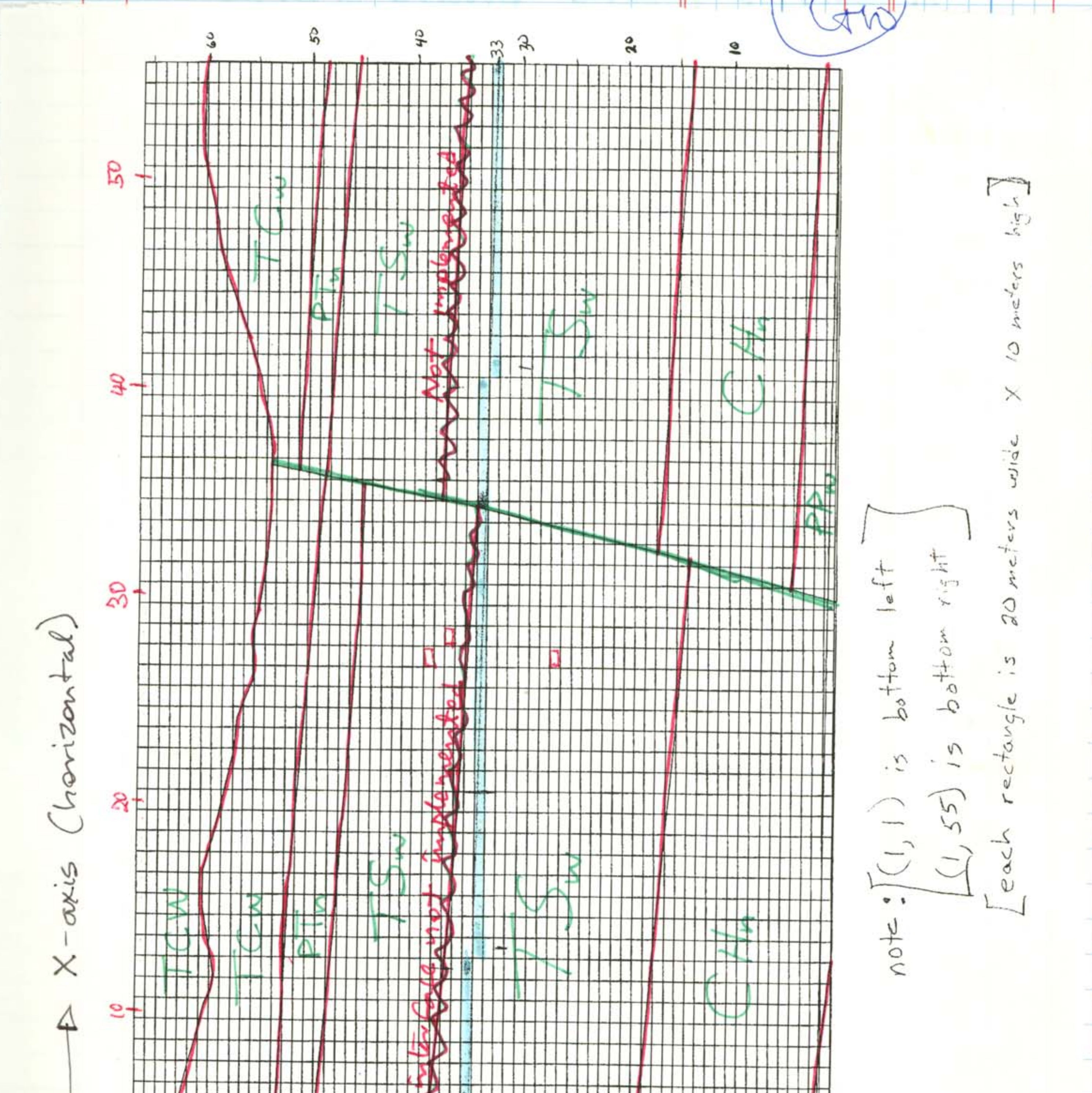
Collaborators: Ronald T Green

Specimen Signatures

Goodluck I Ofoegbu GIO

Problem Geometry:

Stratigraphy extracted digitally from CNWRA Geological Framework Model. The following plot shows the stratigraphic interfaces (red lines), the Ghost-Dance Fault (green) and vertical and horizontal grid lines.



April 22 1996

The grid ~~de~~ discretization shown on page 3 was used for both BIGFLOW (isothermal-flow code) and METRA (nonisothermal-flow code) analyses. The material-index data (which assigns stratigraphic layer number to individual grid cells) was initially setup for BIGFLOW.
Z-axis is positive upward in BIGFLOW but positive downward in METRA. As a result, the material-index data developed for BIGFLOW has to be translated (as will be shown later) to obtain an equivalent material-index data for METRA. The C-code used for the translation is reproduced on the following pages. The code also sets up a database to facilitate transfer of material-property values from BIGFLOW format to METRA format, and preparation of flow-property input block PCKR for METRA. Three codes were used to accomplish the data translation:

matGroups93.c TSPA-93 property set

matGroups95.c TSPA-95 property set

phikTest.c ← This code translates the PHIK ~~inptu~~ input block (prepared using any of the first two codes) into TECPLOT format to enable plotting of the data with TECPLOT to verify that the stratigraphy has been input correctly into METRA.

```
#include <stdio.h>
#include <stdlib.h>

struct BigvGen{
  float n,beta,porosity,mcResid,ksat;
};

main()
{
  char buf[81];
  int i,ix,jy,kz,matNum,numFound;
  int Nx=55,Nz=65,numRockUnits=5;
  int iecm;
  float vb,permeability,fmat;
  float swir,rpm,alpha,pcwmx,sgc;
  float density,viscosity,gravity;
  float n,beta,porosity,mcResid,ksat;
  struct BigvGen **rkUnit,*tcw,*ptn,*tsw,*chn,*ppn;

/**********************************************************************
  matGroups93.c

  This code prepares material-property input block PCKR and
  material-assignment input block PHIK for MULTIFLO. Material parameters
  for 5 rock units are determined using the data structure BigvGen.
  Assignment of rock-unit numbers to finite-difference cells is determined
  using information read from an external file containing material-index
  data extracted from BIGFLOW

  Data structure BigvGen holds the van-Genuchten parameters for a
  rock unit in BIGFLOW format. Material-parameter values are derived from
  TSPA-93 property set.

  n               van Genuchten parameter n
  beta            pressure-head multiplier in van Genuchten function
                  (in units of 1/m)
  porosity        rock-unit porosity
  mcResid         residual moisture content (volumetric ratio)
  ksat            saturated hydraulic conductivity (m/s)

  Author                 G.I. Ofoegbu
  Date                   May 09 1996
  System Requirement     most C compilers will be adequate
**********************************************************************/

/* Initialize material BIGFLOW-format vanGenuchten parameters */

  rkUnit = (struct BigvGen **)malloc(5*sizeof(struct BigvGen *));
  if (!rkUnit)
    DumpAndQuit("Unable to allocate memory for rockUnits array");

  tcw = (struct BigvGen *)malloc(sizeof(struct BigvGen));
  if (!tcw)
    DumpAndQuit("Unable to allocate memory for TCw unit");

  tcw->n = 1.62;
  tcw->beta = 0.0218;
  tcw->porosity = 0.087;
  tcw->mcResid = 0.0018;
  tcw->ksat = 3.86e-10;
  rkUnit[0] = tcw;

  ptn = (struct BigvGen *)malloc(sizeof(struct BigvGen));
  if (!ptn)
    DumpAndQuit("Unable to allocate memory for PTn unit");

  ptn->n = 2.611;
  ptn->beta = 0.2485;
  ptn->porosity = 0.421;
  ptn->mcResid = 0.0648;
  ptn->ksat = 5.47e-7;
  rkUnit[1] = ptn;

  tsw = (struct BigvGen *)malloc(sizeof(struct BigvGen));
  if (!tsw)
    DumpAndQuit("Unable to allocate memory for TCw unit");

  tsw->n = 1.793;
  tsw->beta = 0.0299;
  tsw->porosity = 0.139;
  tsw->mcResid = 0.0063;
  tsw->ksat = 2.37e-10;
  rkUnit[2] = tsw;

  chn = (struct BigvGen *)malloc(sizeof(struct BigvGen));
  if (!chn)
    DumpAndQuit("Unable to allocate memory for CHn unit");

  chn->n = 2.0866;
  chn->beta = 0.0306;
  chn->porosity = 0.319;
  chn->mcResid = 0.0359;
  chn->ksat = 6.22e-9;
  rkUnit[3] = chn;

  ppn = (struct BigvGen *)malloc(sizeof(struct BigvGen));
  if (!ppn)
    DumpAndQuit("Unable to allocate memory for PPn unit");

  ppn->n = 7.014;
  ppn->beta = 0.018;
  ppn->porosity = 0.292;
  ppn->mcResid = 0.0201;
  ppn->ksat = 2.58e-9;
  rkUnit[4] = ppn;

/* Convertion constants */

  density = 1000.0;                /* density of water (kg/m^3) */
  viscosity = 1.0e-3;              /* viscosity of water (Pa.s) */
  gravity = 10;                    /* m/s^2   */

/* Write PCKR input block */

  printf("PCKR\n");
  pcwmx = 0.0;
  sgc = 0.0;
  iecm = 0;

  for (i=0; i<5; i++){
    n = rkUnit[i]->n;
```

```
    beta = rkUnit[i]->beta;
    porosity = rkUnit[i]->porosity;
    mcResid = rkUnit[i]->mcResid;
    swir = mcResid/porosity;
    rpm = 1.0 - 1.0/n;
    alpha = beta/(density*gravity);
    printf("%d  VAN-GEN %12.3e %12.3e %12.3e %5.1f %5.1f %5d\n",
      i+1,swir,rpm,alpha,pcwmx,sgc,iecm);
  }
  printf("0\n");

/* Read material index file and write PHIK input block */

  printf("PHIK\n");
  vb = 0.0;
  jy = 1;
  numFound = 0;

  while (gets(buf))
    if (sscanf(buf,"%d %d %f",&ix,&kz,&fmat) == 3){
      matNum = fmat/1.0e4;
      if (!ix || ix>Nx || !kz || kz>Nz || !matNum || matNum>numRockUnits){
        sprintf(buf,"Invalid input: ix=%d kz=%d matNum=%d",ix,kz,matNum);
        DumpAndQuit(buf);
      }
      i = matNum-1;
      porosity = rkUnit[i]->porosity;
      ksat = rkUnit[i]->ksat;
      permeability = ksat*viscosity/(density*gravity);
      printf("%5d%5d%5d%5d%5d%5d%3d%3d%5.1f%10.4f%12.3e%12.3e%12.3e\n",
        ix,ix,jy,jy,Nz-kz+1,Nz-kz+1,
        matNum,matNum,
        vb,
        porosity,permeability,permeability,permeability
      );
      numFound++;
    }

  printf("0\n");
  if (numFound != Nx*Nz)
    printf("\n\n *** Material assignment found for %d of expected %d cells\n\n",
      numFound,Nx*Nz);
}

DumpAndQuit(s)
char *s;
{
  printf("\n *** %s ***\n\n",s);
  exit(0);
}
```

```c
#include <stdio.h>
#include <stdlib.h>

struct BigvGen{
  float n,beta,porosity,mcResid,ksat;
};

main()
{
  char buf[81];
  int i,ix,jy,kz,matNum,numFound;
  int Nx=55,Nz=65,numRockUnits=5;
  int iecm;
  float vb,permeability,fmat;
  float swir,rpm,alpha,pcwmx,sgc;
  float density,viscosity,gravity;
  float n,beta,porosity,mcResid,ksat;
  struct BigvGen **rkUnit,*tcw,*ptn,*tsw,*chnv,*chnz;

/***************************************************************************
  matGroups95.c

  This code prepares material-property input block PCKR and
  material-assignment input block PHIK for MULTIFLO. Material parameters
  for 5 rock units are determined using the data structure BigvGen.
  Assignment of rock-unit numbers to finite-difference cells is determined
  using information read from an external file containing material-index
  data extracted from BIGFLOW

  Data structure BigvGen holds the van-Genuchten parameters for a
  rock unit in BIGFLOW format. Material-parameter values are derived from
  TSPA-95 property set.

  n                  van Genuchten parameter n
  beta               pressure-head multiplier in van Genuchten function
                     (in units of 1/m)
  porosity           rock-unit porosity
  mcResid            residual moisture content (volumetric ratio)
  ksat               saturated hydraulic conductivity (m/s)

  Author                    G.I. Ofoegbu
  Date                      May 09 1996
  System Requirement        most C compilers will be adequate
***************************************************************************/

/* Initialize material BIGFLOW-format vanGenuchten parameters */

  rkUnit = (struct BigvGen **)malloc(5*sizeof(struct BigvGen *));
  if (!rkUnit)
    DumpAndQuit("Unable to allocate memory for rockUnits array");

  tcw = (struct BigvGen *)malloc(sizeof(struct BigvGen));
  if (!tcw)
    DumpAndQuit("Unable to allocate memory for TCw unit");

  tcw->n = 1.558;
  tcw->beta = 0.0084;
  tcw->porosity = 0.087;
  tcw->mcResid = 1.74e-4;
  tcw->ksat = 9.7e-12;
  rkUnit[0] = tcw;

  ptn = (struct BigvGen *)malloc(sizeof(struct BigvGen));
  if (!ptn)
    DumpAndQuit("Unable to allocate memory for PTn unit");

  ptn->n = 6.872;
  ptn->beta = 0.0153;
  ptn->porosity = 0.421;
  ptn->mcResid = 0.0421;
  ptn->ksat = 3.9e-7;
  rkUnit[1] = ptn;

  tsw = (struct BigvGen *)malloc(sizeof(struct BigvGen));
  if (!tsw)
    DumpAndQuit("Unable to allocate memory for TCw unit");

  tsw->n = 1.798;
  tsw->beta = 0.0058;
  tsw->porosity = 0.139;
  tsw->mcResid = 1.112e-2;
  tsw->ksat = 1.9e-11;
  rkUnit[2] = tsw;

  chnv = (struct BigvGen *)malloc(sizeof(struct BigvGen));
  if (!chnv)
    DumpAndQuit("Unable to allocate memory for CHnv unit");

  chnv->n = 3.861;
  chnv->beta = 0.0163;
  chnv->porosity = 0.331;
  chnv->mcResid = 1.3571e-2;
  chnv->ksat = 2.7e-7;
  rkUnit[3] = chnv;

  chnz = (struct BigvGen *)malloc(sizeof(struct BigvGen));
  if (!chnz)
    DumpAndQuit("Unable to allocate memory for CHnz unit");

  chnz->n = 1.602;
  chnz->beta = 0.0031;
  chnz->porosity = 0.306;
  chnz->mcResid = 3.366e-2;
  chnz->ksat = 2.0e-11;
  rkUnit[4] = chnz;

/* Convertion constants */

  density = 1000.0;                 /* density of water (kg/m^3) */
  viscosity = 1.0e-3;               /* viscosity of water (Pa.s) */
  gravity = 10;                     /* m/s^2   */

/* Write PCKR input block */

  printf("PCKR\n");
  pcwmx = 0.0;
  sgc = 0.0;
  iecm = 0;

  for (i=0; i<5; i++){
    n = rkUnit[i]->n;
```

```
    beta = rkUnit[i]->beta;
    porosity = rkUnit[i]->porosity;
    mcResid = rkUnit[i]->mcResid;
    swir = mcResid/porosity;
    rpm = 1.0 - 1.0/n;
    alpha = beta/(density*gravity);
    printf("%d  VAN-GEN %12.3e %12.3e %12.3e %5.1f %5.1f %5d\n",
      i+1,swir,rpm,alpha,pcwmx,sgc,iecm);
  }
  printf("0\n");

/* Read material index file and write PHIK input block */

  printf("PHIK\n");
  vb = 0.0;
  jy = 1;
  numFound = 0;

  while (gets(buf))
    if (sscanf(buf,"%d %d %f",&ix,&kz,&fmat) == 3){
      matNum = fmat/1.0e4;
      if (!ix || ix>Nx || !kz || kz>Nz || !matNum || matNum>numRockUnits){
        sprintf(buf,"Invalid input: ix=%d kz=%d matNum=%d",ix,kz,matNum);
        DumpAndQuit(buf);
      }
      i = matNum-1;
      porosity = rkUnit[i]->porosity;
      ksat = rkUnit[i]->ksat;
      permeability = ksat*viscosity/(density*gravity);
      printf("%5d%5d%5d%5d%5d%5d%5d%3d%3d%5.1f%10.4f%12.3e%12.3e%12.3e\n",
        ix,ix,jy,jy,Nz-kz+1,Nz-kz+1,
        matNum,matNum,
        vb,
        porosity,permeability,permeability,permeability
      );
     numFound++;
    }

  printf("0\n");
  if (numFound != Nx*Nz)
    printf("\n\n *** Material assignment found for %d of expected %d cells\n\n",
      numFound,Nx*Nz);
}

DumpAndQuit(s)
char *s;
{
  printf("\n *** %s ***\n\n",s);
  exit(0);
}
```

```
#include <stdio.h>

main()
{
  char buf[121];
  int ix,kz,matnum,dx=20,dz=10;

/*****************************************************************
  phikTest.c

  This code converts a PHIK input block (prepared for METRA)
  into a tecplot format to enable verification of the PHIK input
  block (through a tecplot plot)

  Author:                      G.I. Ofoegbu
  Date:                        May 15 1996
  System Requirement:          ANSI C
                               (Compile with acc on SUN OS platform)

*****************************************************************/

  printf(" zone  i=  55 j=  65\n");

  while (gets(buf))
    if (sscanf(buf,"%d %*d %*d %*d %d %*d %d %*d %*f",
    &ix,&kz,&matnum) == 3)
      printf("%10d%10d%10d\n",ix*dx,-kz*dz,matnum);
}
```

Sample Input File (Isothermal Analyses)

Listing for **Goodluck Ofoegbu**

```
Example 2D Perched-Water Problem
Case 08: Infiltration equal to TC Ksat; initial saturation of 25%
RSTART 0
:
: Grid definition
:
GRID XYZ 55 1 65 0 1 1
DXYZ 0
20.0
1.0
10.0
:
: Material-properties definition and assignment to grid blocks
:
THERM
: no rho        cpr    ckdry  cksat    crp  crt    tau  cdiff    cexp  enbd
  1  2.580e+03 840.0  1.74     2.3     0    0     .0  2.13e-5  1.8    1.
  2  2.580e+03 840.0  1.74     2.3     0    0     .0  2.13e-5  1.8    1.
  3  2.580e+03 840.0  1.74     2.3     0    0     .0  2.13e-5  1.8    1.
  4  2.580e+03 840.0  1.74     2.3     0    0     .0  2.13e-5  1.8    1.
  5  2.580e+03 840.0  1.74     2.3     0    0     .0  2.13e-5  1.8    1.
0
PCKR
1  VAN-GEN    2.000e-03    3.582e-01    8.400e-07   0.0   0.0     0
2  VAN-GEN    1.000e-01    8.545e-01    1.530e-06   0.0   0.0     0
3  VAN-GEN    8.000e-02    4.438e-01    5.800e-07   0.0   0.0     0
4  VAN-GEN    4.100e-02    7.410e-01    1.630e-06   0.0   0.0     0
5  VAN-GEN    1.100e-01    3.758e-01    3.100e-07   0.0   0.0     0
0
PHIK  c05          : Get material assignments from c05.phk
:
: Initial conditions
:
INIT
    1   55    1    1     1   64   1.0725e+05    25.000   0.75      0   0
    1   55    1    1    65   65   1.0725e+05    25.000   0.0001   0   0
0
MONItor
1512 1623 2172
RECUrrent-data
:
OUTPUT P=1 L=1 T=1
SOLVE   4   4   12
:
:TOLR TOLP  TOLS  TOLT  TOLP2  TOLM  TOLA  TOLE
Tolr  1.e-1 1.e-5 1.e-4 1.e+0  1.e-6 1.e-6 1.e-6 1.e-20 1.e-20 1.e-20
:
:Limit dpmx dsmx dtmpmx dp2mx dtmn    dtmx icutmx
LIMIT  5.e6 .07    7.    5.e5  1.e-7   1.e3  0
:
:AUTO-step  DPMXE    DSMXE DTMPMXE DP2MXe TACCEL IAUTO
AUTO-step   1.0E+5   0.03    3.0    1.e30
Plots 1
:
: Boundary conditions
:
BCON 2
  1 BOTTOM 1 55 1 1
  0   0  1.0725E5 25.0 0.0001 0
0
  3 TOP    1 55 1 1
  0    3.059E-4 1.0 25 0.0001 0
0
RSTART 1
STEADY[y] 1.0
ENDS
```

(GW)

A sample input file is shown above. As the file shows, an initial water saturation of 0.25 was applied everywhere, water-table conditions (atmospheric pressure and ~~small~~ negligible gas saturation) were applied at the base of the model, and a steady downward infiltration of 0.3 mm/yr was applied at the top. The vertical boundaries of the model are no-flow boundaries (by default). The model was set to run to steady state, which was defined as water pressure (or gas pressure) change of 1.0 Pa/yr or less.

Sample Input File (Nonisothermal Analyses)

Listing for **Goodluck Ofoegbu**

```
Example 2D Perched-Water Problem with thermal perturbation
Case 10: Steady-state solution of Case 08 as initial condition
RSTART 0
:
: Grid definition
:
GRID XYZ 55 1 65 0 1 1
DXYZ 0
20.0
1.0
10.0
:
: Material-properties definition and assignment to grid blocks
:
THERM
: no rho        cpr    ckdry  cksat    crp  crt    tau  cdiff    cexp  enbd
  1  2.580e+03 728.0  1.69    2.23     0    0      .5  2.13e-5  1.8    1.
  2  2.580e+03 422.0  0.61    0.81     0    0      .5  2.13e-5  1.8    1.
  3  2.580e+03 840.0  2.10    2.78     0    0      .0  2.13e-5  1.8    1.
  4  2.580e+03 488.0  0.84    1.11     0    0      .0  2.13e-5  1.8    1.
  5  2.580e+03 526.0  0.42    1.88     0    0      .0  2.13e-5  1.8    1.
0
PCKR
1  VAN-GEN    2.000e-03    3.582e-01    8.400e-07   0.0   0.0     0
2  VAN-GEN    1.000e-01    8.545e-01    1.530e-06   0.0   0.0     0
3  VAN-GEN    8.000e-02    4.438e-01    5.800e-07   0.0   0.0     0
4  VAN-GEN    4.100e-02    7.410e-01    1.630e-06   0.0   0.0     0
5  VAN-GEN    1.100e-01    3.758e-01    3.100e-07   0.0   0.0     0
0
PHIK  c05          : Get material assignments from c05.phk
INIT c08out        : Get initial conditions from c08out.int
:
: MONItor
: 1512 1623 2172
RECUrrent-data
:
OUTPUT P=1 L=1 T=1
SOLVE   4   4   12
:
:TOLR TOLP  TOLS  TOLT  TOLP2  TOLM  TOLA  TOLE
Tolr  1.e-1 1.e-5 1.e-4 1.e+0  1.e-6 1.e-6 1.e-6 1.e-20 1.e-20 1.e-20
:
:Limit dpmx dsmx dtmpmx dp2mx dtmn    dtmx icutmx
LIMIT  5.e6 .07    7.   5.e5  1.e-7   1.e3  0
:
:AUTO-step  DPMXE    DSMXE DTMPMXE DP2MXe TACCEL IAUTO
AUTO-step   1.0E+5   0.03    3.0    1.e30
Plots 1
SOURCE  1  1.0  1.0  qh83   : read heat source definition from qh83.src
:
: Boundary conditions
:
BCON 2
  1 BOTTOM 1 55 1 1
  0   0  1.0725E5 25.0 0.0001 0
0
  3 TOP     1 55 1 1
  0   3.059E-4 1.0 25 0.0001 0
0
: RSTART 1
TIME[y] 100.
ENDS
```

The noinisothermal analyses differ from the isothermal as follows:

(1) The results of the isothermal analysis were used to define the initial conditions for the nonisothermal

(2) A time-varying heat source was applied over selected cells (entire row of cells along K=34) to simulate repository heating

(3) Each analysis was run to specified time (the isothermal was run to steady state).

The strength of the heat source was ~~defi~~ given in terms of the heat flux q (J/s) that emanates from a grid cell, which was calculated as follows:

$$q = Q N_{wp} \left(\frac{A_{cell}}{A_{wp}} \right)$$

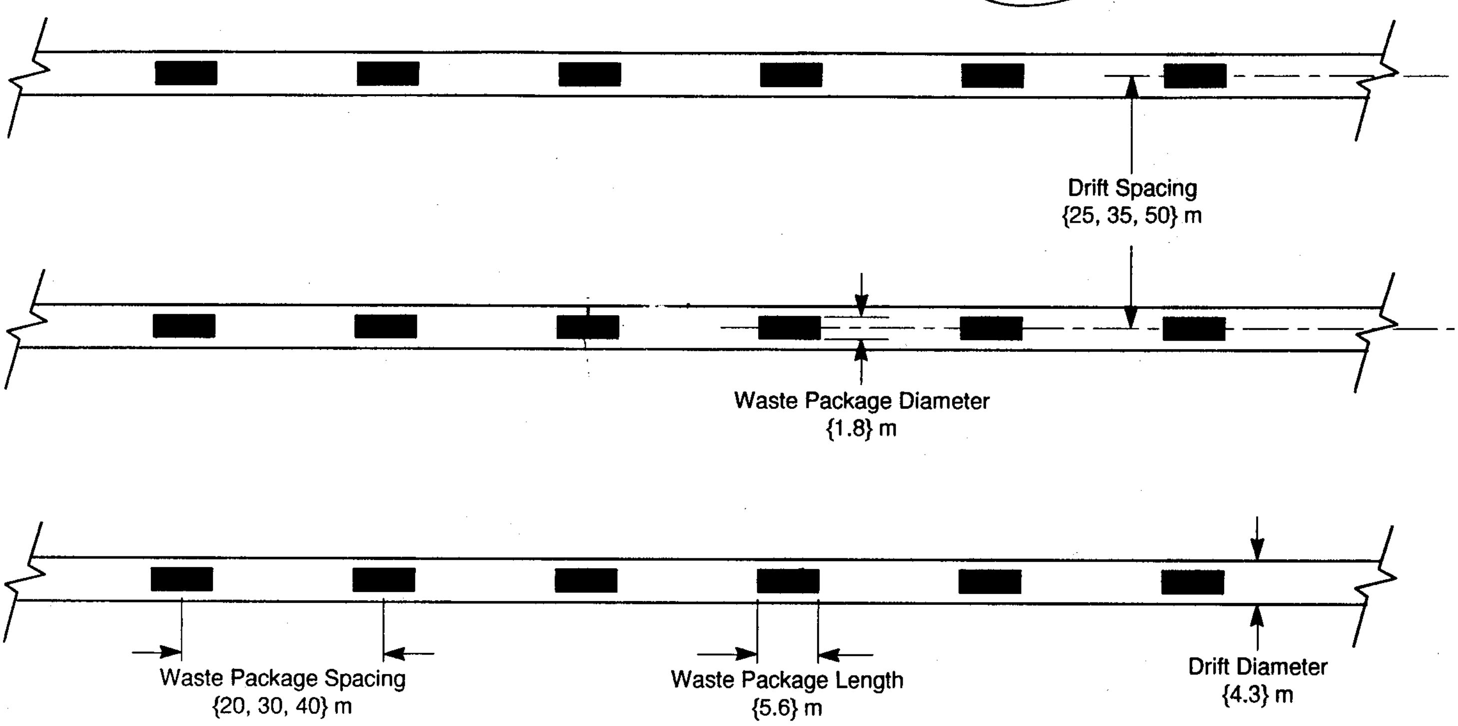
where

$N_{wp} = 8.8$ = number of MTU's (metric tons of uranium) in one waste package.

A_{cell} = area of a grid cell = 20 m^2 per m section

A_{wp} = tributary area assigned to a waste package, which depends on the waste-package spacing and drift spacing, as shown in the figure below. For the case of 83 MTU/acre thermal loading,

$$A_{wp} = 19 \times 22 \ m^2$$



Q = heat flux due to 1 MTU.

Q is a time function computed based on DOE's

recommendations (Characteristics of spent fuel, high-level wastes which may require long-term isolation. DOE/RW-0184, Vol. 2. Washington D.C., U.S. Department of Energy, 1987). The computation ~~was~~ of Q was coded in a FORTRAN Subroutine by R. D. Manteufel.

The computation of q using the above equation was implemented using the FORTRAN code below, which outputs its results in the format required for input to METRA.

(GIO)

```
      IMPLICIT REAL*8(A-H,O-Z)
C
C     Code HeatSrcByArea computes transient heat flux (J/s) emanating from
C     an area (ACELL) of the repository. The heat flux (J/s) due to
C     1 MTU (FLUX) is computed in subroutine MTUFLX (developed by
C     R. D. Mantuefel) and is multiplied by the number of MTUs per waste
C     package (WPMTU) and divided by the waste-package tributary are
C     (AWP) to obtain the flux per unit area for the repository, which is
C     then multiplied by ACELL to obtain the total flux that emanates
C     from ACELL. The case illustrated is for an 83 MTU/acre thermal-load
C     option, for which the waste-package spacing (WPSP) and the drift
C     spacing (DRFTSP) are 19 and 22 m, respectively.
C
C     Author:     G. I. Ofoegbu
C     Date:       June 12 1996
C
      WPSP = 19.0
      DRFTSP = 22.0
      WPMTU = 8.8
      ACELL = 20.0
      AWP = WPSP*DRFTSP
C
      TIME = 0.0
C
  100 CALL MTUFLX(FLUX,TIME)
      TSEC = TIME*365.0*24.0*3600.0
      CELFLX = (FLUX*WPMTU/AWP)*ACELL
      WRITE(6,1000) TSEC,CELFLX
      DT = 0.1
      IF (TIME .GT. 1.0) DT = 0.5
      IF (TIME .GT. 10.0) DT = 5.0
      IF (TIME .GT. 100.0) DT = 50.0
      IF (TIME .GT. 1000.0) DT = 500.0
      TIME = TIME + DT
      IF (TIME .LT. 10010.0) GO TO 100
      STOP
 1000 FORMAT(2E12.3)
      END
      SUBROUTINE MTUFLX( FLUX, TIME)
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION TIMES(38), PWR(38), BWR(38)
C
      DATA TIMES / 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0,
     1 16.0, 18.0, 20.0, 25.0, 30.0, 40.0, 50.0, 60.0, 70.0, 80.0,
     1 90.0, 100.0, 200.0, 300.0, 400.0, 500.0, 1000.0, 2000.0,
     1 3000.0, 5000.0, 10000.0, 30000.0, 40000.0, 50000.0, 100000.0,
     1 200000.0, 500000.0, 1000000.0 /
C
C PWR WITH 42 GWD/MTU BURNUP
      DATA PWR / 10582.390, 5740.4059, 3759.2845, 2784.2818,
     1  2265.6947, 1957.4007, 1769.3468, 1641.4306, 1547.4025,
     1  1477.2287, 1231.4270, 1177.4945, 1133.5847, 1026.9513,
     1  941.70979, 796.60790, 682.24662, 591.08155, 531.67177,
     1  458.53320, 410.13654, 371.14194, 205.60656, 159.43532,
     1  134.23410, 116.03889, 65.483382, 33.112897, 25.230178,
     1  20.668519, 15.006216, 5.9303608, 4.2836496, 3.2613031,
     1  1.2804850, 0.80268576, 0.67173300, 0.48635582 /
C
C BWR WITH 32 GWD/MTU BURNUP
      DATA BWR / 6648.7963, 3652.6734, 2437.5396, 1834.6740,
     1  1522.4266, 1334.2946, 1226.4492, 1142.4117, 1088.4892,
     1  1045.2362, 887.48326, 851.11466, 817.75730, 744.64654,
     1  682.32031, 577.22915, 494.33762, 427.36371, 373.44121,
     1  329.67049, 294.30397, 265.33367, 146.33258, 115.24506,
     1  98.253661, 85.614640, 50.235460, 27.102957, 21.205846,
     1  17.606008, 12.704777, 4.9260472, 3.5334570, 2.6730881,
     1  1.0138927, 0.60454605, 0.50774771, 0.37405906 /
C
C AVG BURNUP = 38.5 GWD/MTU
C
C Apply heat flux to canister
C
            AGE = 23.0
C
            TYR = TIME + AGE
C
            IF( TYR .LT. TIMES(1) ) THEN
              TYR = TIMES(1) + 1.0D-8
            ELSEIF( TYR .GT. TIMES(38) ) THEN
              TYR = TIMES(38) - 1.0D-8
            ENDIF
C
            DO I = 1, 38
              IF( TYR .LT. TIMES(I) ) THEN
                J = I - 1
                GOTO 8833
              ENDIF
            ENDDO
            J = 37
 8833       CONTINUE
C
            AM = DLOG(PWR(J)/PWR(J+1)) / DLOG(TIMES(J+1)/TIMES(J))
            QP = PWR(J) * (TIMES(J) / TYR )**AM
C
            AM = DLOG(BWR(J)/BWR(J+1)) / DLOG(TIMES(J+1)/TIMES(J))
            QB = BWR(J) * (TIMES(J) / TYR )**AM
C
            QWP  = 0.65*QP + 0.35*QB
C
            FLUX = QWP
         RETURN
         END
```

The output from the FORTRAN code can also be plotted using XPLOT (or any other x-y plotting program), to enable verification of the heat input.

An alternative approach for calculating the heat flux ~~vs~~ q was also examined, which is based on the following equation

$$q = \frac{V_{cell}}{V_{rep}} \times M_t Q$$

where

$$V_{rep} = (\Delta t) \times \frac{M_t}{M_a}$$

V_{cell} = volume of a cell, which, for a vertical 2D section, is equal to $\Delta t . A_{cell}$, where A_{cell} is as defined earlier.

V_{rep} = repository volume

M_t = Total number of metric tons of uranium to be stored at the repository = 63000.0

Δt = Thickness of the repository (vertical thickness)

M_a = Number of metric tons of uranium per unit area, which depends on the thermal-load option (e.g. 83 MTU/acre)

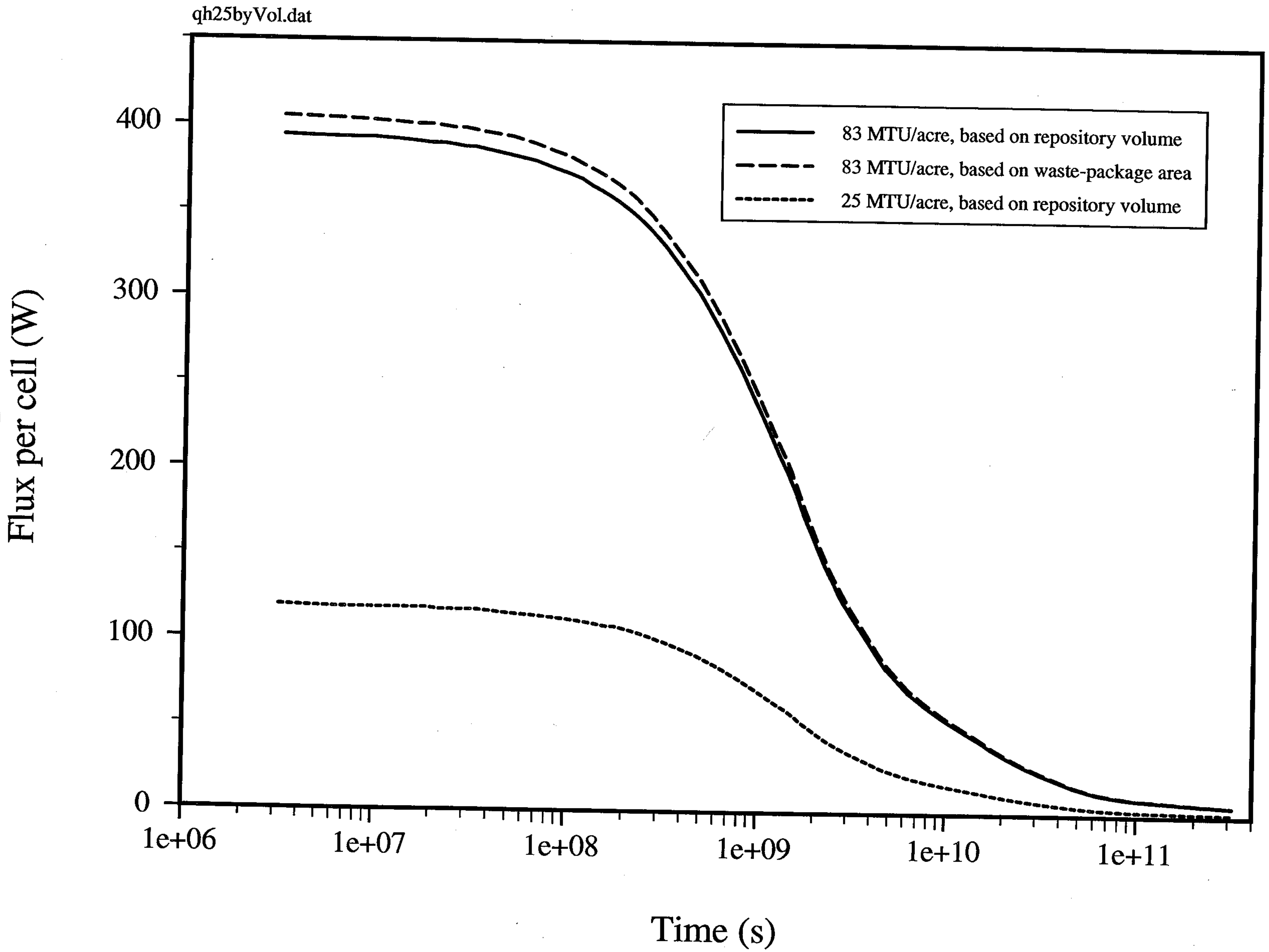
(Note: 1 acre = 4047 m^2)

The implementation of the volume-based approach was through the FORTRAN code reproduced on the next page, which also uses the subroutine MTUFLX to compute Q.

Heat flux ~~distributions~~ (G10) vs time functions computed using the area-based and volume-based formulas are essentially the same, as is shown in the following figure (p. 15). The area-based formula was used for subsequent calculations.

```
      IMPLICIT REAL*8(A-H,O-Z)
C
C     Code HeatSrcByVol computes transient heat flux (J/s) emanating from
C     a volume (VCELL) of the repository. The heat flux (J/s) due to
C     1 MTU (FLUX) is computed in subroutine MTUFLX (developed by
C     R. D. Mantuefel) and is multiplied by the number of MTUs in the
C     repository (TMTU) and divided by the repository volume (VREPO)
C     to obtain the average flux per unit repository volume (FLXPV),
C     which is multiplied by VCELL to obtain the total flux that emanates
C     from VCELL. The repository is model as a 10-m thick slab, and the
C     case illustrated is for an 83 MTU/acre thermal loading.
C
C     Author:     G. I. Ofoegbu
C     Date:       June 12 1996
C
      ACRE = 4047.0
      THICK = 10.0
      AML = 83.0
      TMTU = 63000.0
      VCELL = 20.0*10.0
      AREA = ACRE*TMTU/AML
      VREPO = AREA*THICK
C
      TIME = 0.0
C
  100 CALL MTUFLX(FLUX,TIME)
      TSEC = TIME*365.0*24.0*3600.0
      FLXPV = TMTU*FLUX/VREPO
      CELFLX = VCELL*FLXPV
      WRITE(6,1000) TSEC,CELFLX
      DT = 0.1
      IF (TIME .GT. 1.0) DT = 0.5
      IF (TIME .GT. 10.0) DT = 5.0
      IF (TIME .GT. 100.0) DT = 50.0
      IF (TIME .GT. 1000.0) DT = 500.0
      TIME = TIME + DT
      IF (TIME .LT. 10010.0) GO TO 100
      STOP
 1000 FORMAT(2E12.3)
      END
      SUBROUTINE MTUFLX( FLUX, TIME)
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION TIMES(38), PWR(38), BWR(38)
C
      DATA TIMES / 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0,
     1 16.0, 18.0, 20.0, 25.0, 30.0, 40.0, 50.0, 60.0, 70.0, 80.0,
     1 90.0, 100.0, 200.0, 300.0, 400.0, 500.0, 1000.0, 2000.0,
     1 3000.0, 5000.0, 10000.0, 30000.0, 40000.0, 50000.0, 100000.0,
     1 200000.0, 500000.0, 1000000.0 /
C
C PWR WITH 42 GWD/MTU BURNUP
      DATA PWR / 10582.390, 5740.4059, 3759.2845, 2784.2818,
     1  2265.6947, 1957.4007, 1769.3468, 1641.4306, 1547.4025,
     1  1477.2287, 1231.4270, 1177.4945, 1133.5847, 1026.9513,
     1  941.70979, 796.60790, 682.24662, 591.08155, 531.67177,
     1  458.53320, 410.13654, 371.14194, 205.60656, 159.43532,
     1  134.23410, 116.03889, 65.483382, 33.112897, 25.230178,
     1  20.668519, 15.006216, 5.9303608, 4.2836496, 3.2613031,
     1  1.2804850, 0.80268576, 0.67173300, 0.48635582 /
C
C BWR WITH 32 GWD/MTU BURNUP
      DATA BWR / 6648.7963, 3652.6734, 2437.5396, 1834.6740,
     1  1522.4266, 1334.2946, 1226.4492, 1142.4117, 1088.4892,
     1  1045.2362, 887.48326, 851.11466, 817.75730, 744.64654,
     1  682.32031, 577.22915, 494.33762, 427.36371, 373.44121,
     1  329.67049, 294.30397, 265.33367, 146.33258, 115.24506,
     1  98.253661, 85.614640, 50.235460, 27.102957, 21.205846,
     1  17.606008, 12.704777, 4.9260472, 3.5334570, 2.6730881,
     1  1.0138927, 0.60454605, 0.50774771, 0.37405906 /
C
C AVG BURNUP = 38.5 GWD/MTU
C
C Apply heat flux to canister
C
          AGE = 23.0
C
          TYR = TIME + AGE
C
          IF( TYR .LT. TIMES(1) ) THEN
            TYR = TIMES(1) + 1.0D-8
          ELSEIF( TYR .GT. TIMES(38) ) THEN
            TYR = TIMES(38) - 1.0D-8
          ENDIF
C
          DO I = 1, 38
            IF( TYR .LT. TIMES(I) ) THEN
              J = I - 1
              GOTO 8833
            ENDIF
          ENDDO
          J = 37
 8833     CONTINUE
C
          AM = DLOG(PWR(J)/PWR(J+1)) / DLOG(TIMES(J+1)/TIMES(J))
          QP = PWR(J) * (TIMES(J) / TYR )**AM
C
          AM = DLOG(BWR(J)/BWR(J+1)) / DLOG(TIMES(J+1)/TIMES(J))
          QB = BWR(J) * (TIMES(J) / TYR )**AM
C
          QWP  = 0.65*QP + 0.35*QB
C
          FLUX = QWP
      RETURN
      END
```

Cell Flux for 20 m by 10 m Cells



June 10 1996

Results

Under the influence of a constant infiltration flux of 0.3 mm/yr and isothermal conditions the flow system exhibited the following behavior. The PTn unit, having a high permeability, allows water to flow freely down through it. When it encounters the TSw unit, which has a low permeability, its downward flow is inhibited. This causes the water to be channelled downdip in the PTn until it reaches the GDF. The footwall of the fault has been uplifted such that the PTn in the hanging wall is juxtaposed against the relatively impermeable TSw unit in the footwall of the fault. This produces a trap where the water that is channelled downdip through the PTn encounters the relatively impermeable TSw at the fault and begins to accumulate, producing a perched water body. As it continues to accumulate, it percolates slowly downward through the TSw unit, thus extending the perched water body well in the TSw unit. The perched body continues to grow as long as there is enough water above it to supply it with water faster than it can be dissipated and reaches a steady-state condition that is characterized by very high saturation values (99% and higher) immediately updip of the GDF ~~(Figure 1a).~~ GW See figure on next page. (18–19)

The isothermal results are used as initial condition for the nonisothermal analysis. Almost immediately (in one year or less), the effects of repository heating are felt in terms of increased saturation and liquid- and gas-phase velocities at the level of the repository ~~(Figure 1 a,b,c)~~ GW on pp. 18, 19. It is worthwhile noting that this is particularly amplified below the area of ~~highest~~ saturation values predicted under the isothermal conditions. As time progresses, a high saturation zone develops at the repository depth, immediately updip of the GDF. This perched water volume increases with time, reaches a maximum value, and then starts dissipating under the influence of elevated temperatures, until it finally breaks down after 250 yrs, and ultimately completely dries out after approximately 1,000 yrs. Representative snapshots of the saturation contours are depicted in ~~Figure 2.~~ GW figures on pages 20, 21 and 22.

Figure on This Page

Results of nonisothermal analyses after 1 yr of repository heating with steady-state isothermal analysis results as initial conditions. Solid white lines represent stratigraphic structure and topography. Dashed black lines correspond to steady-state (isothermal analysis) saturation values.

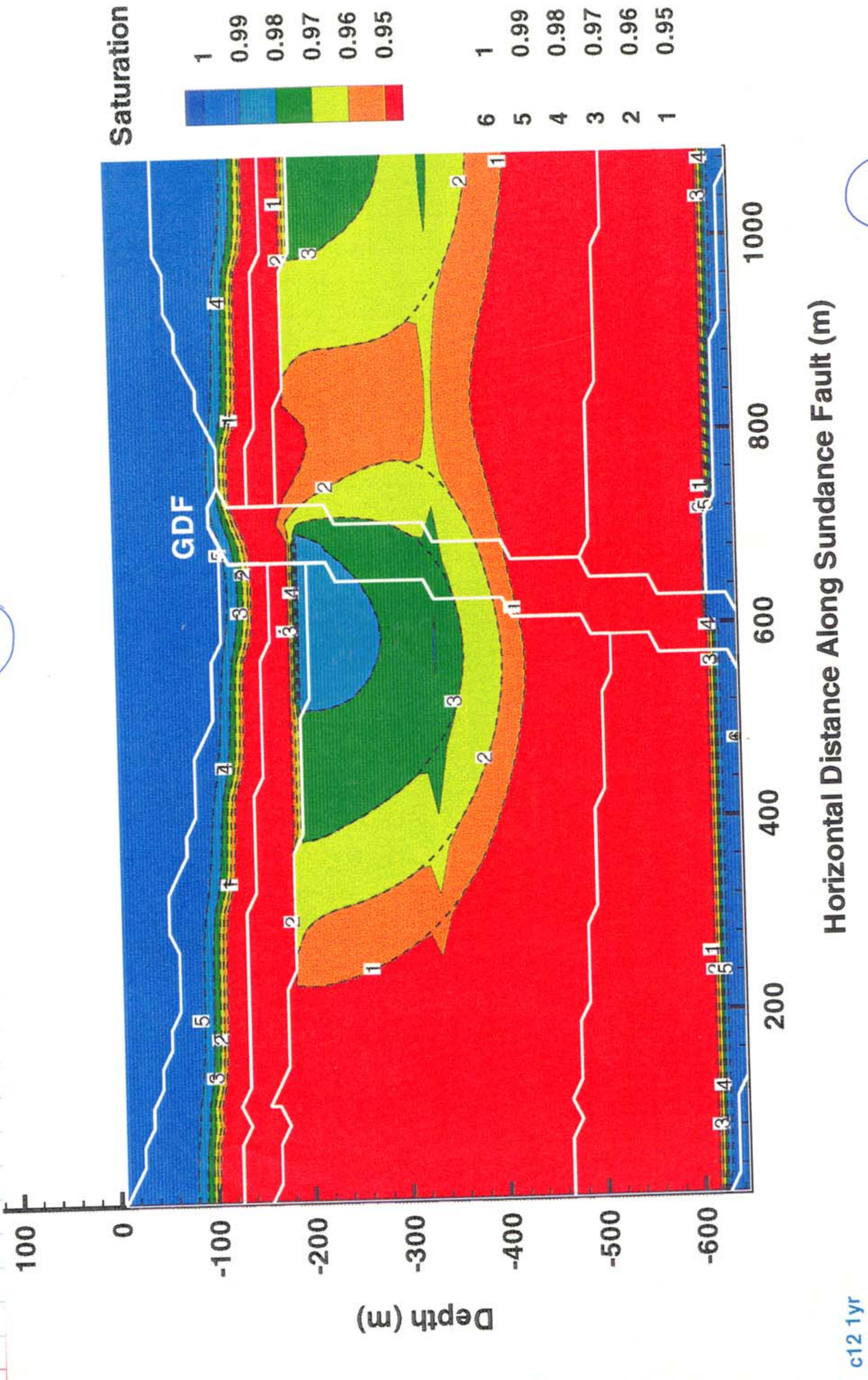


Figure on This Page

Liquid-phase velocity for analysis results shown on Page 17 (nonisothermal case)

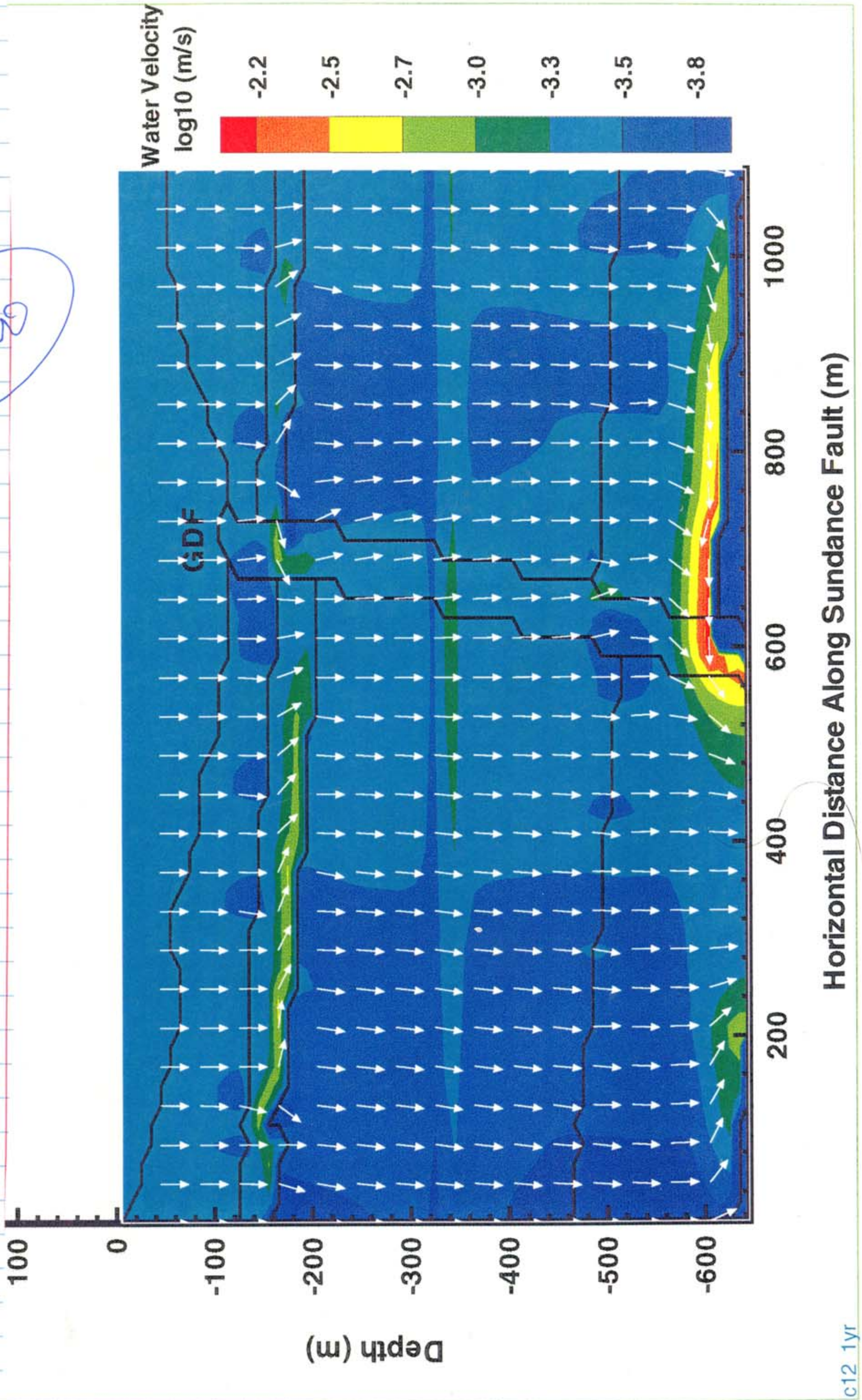


Figure on This Page

Gas-phase velocity for analysis results shown on Page 17 (nonisothermal case).

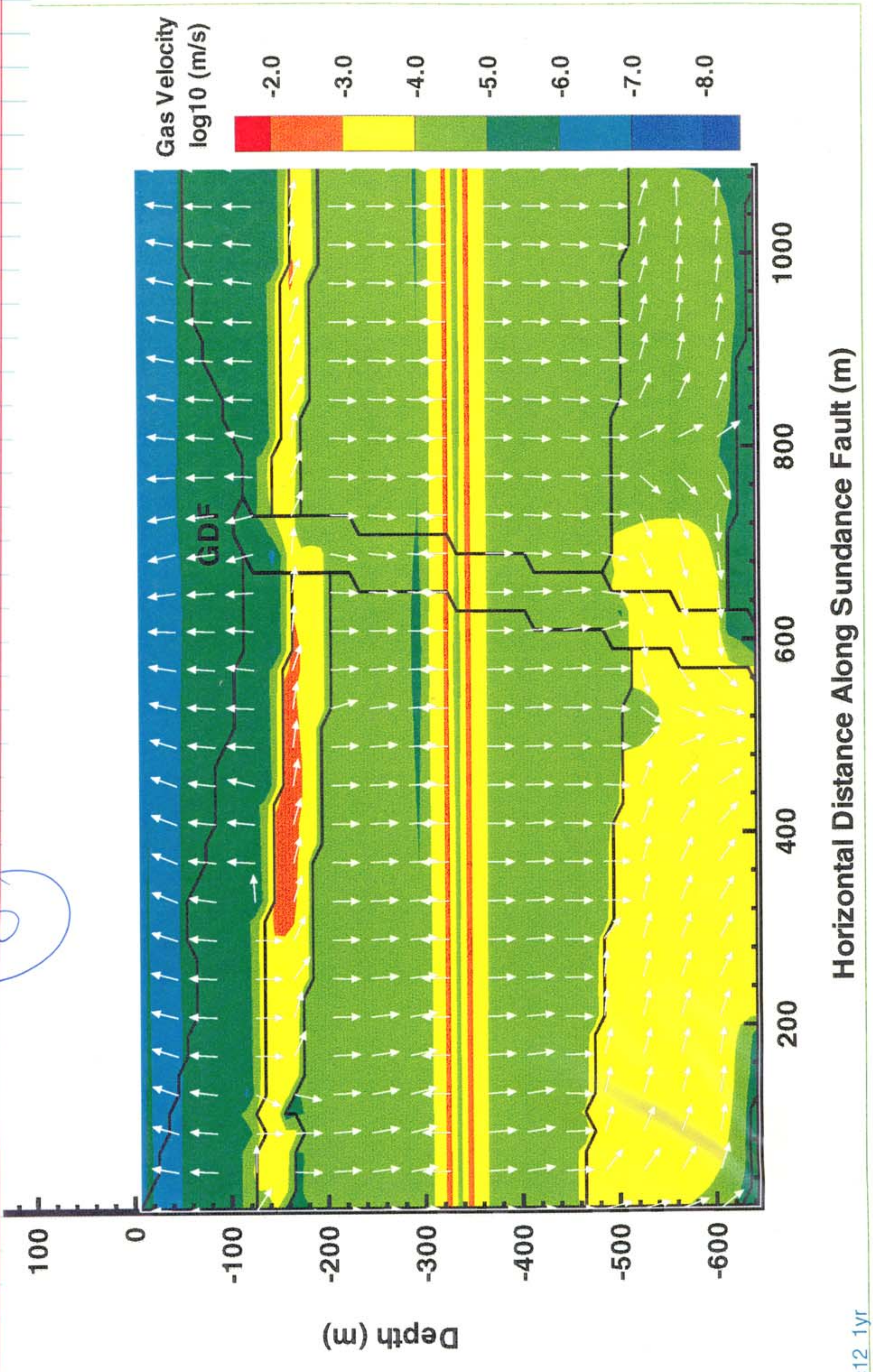


Figure on This Page

Saturation contours at 20 yrs following start of repository heating. Dashed, black lines correspond to steady-state saturation base on isothermal analysis.

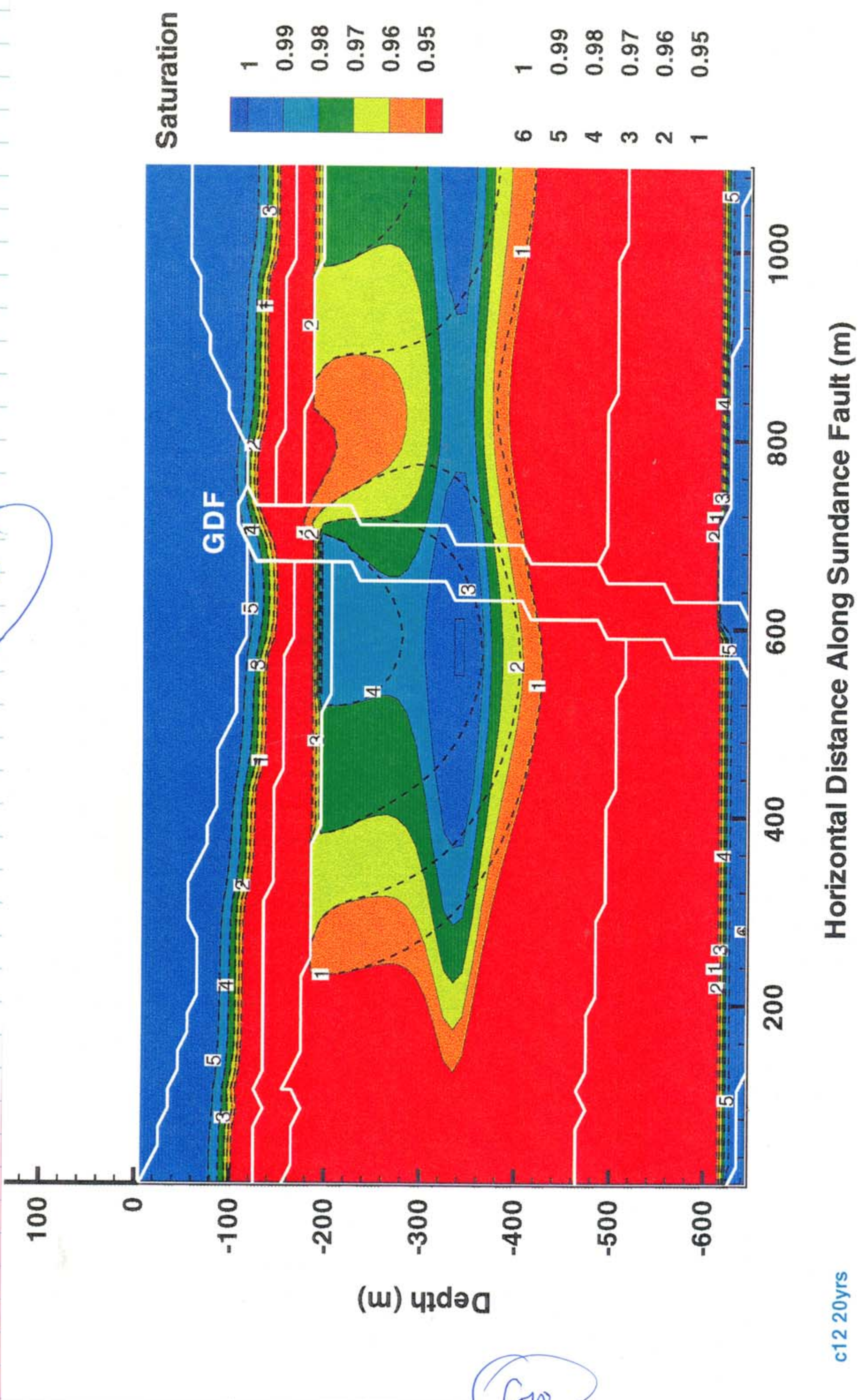


Figure on This Page

Same as on Page 20, except this page is for 100 yrs following start of repository heating.

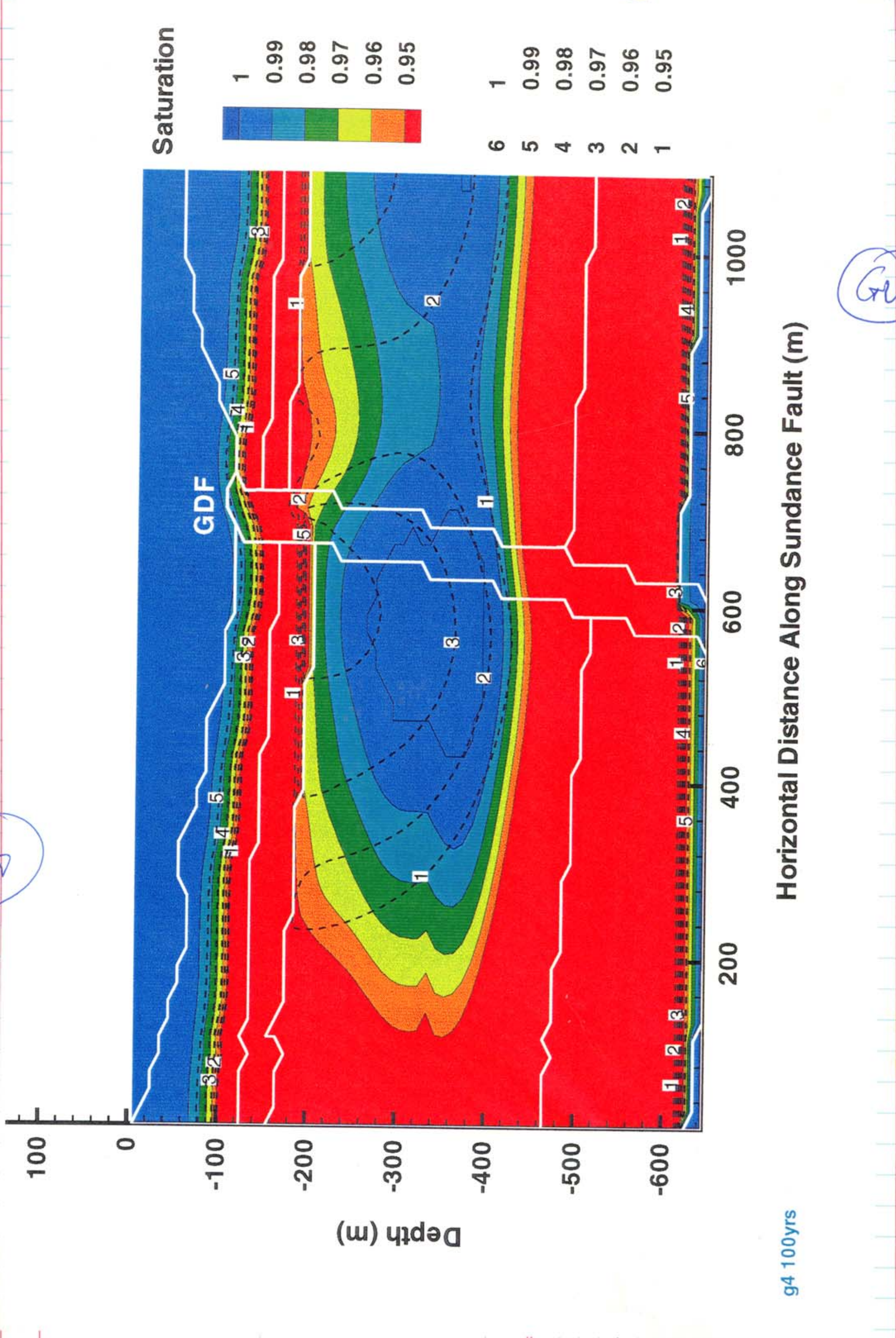
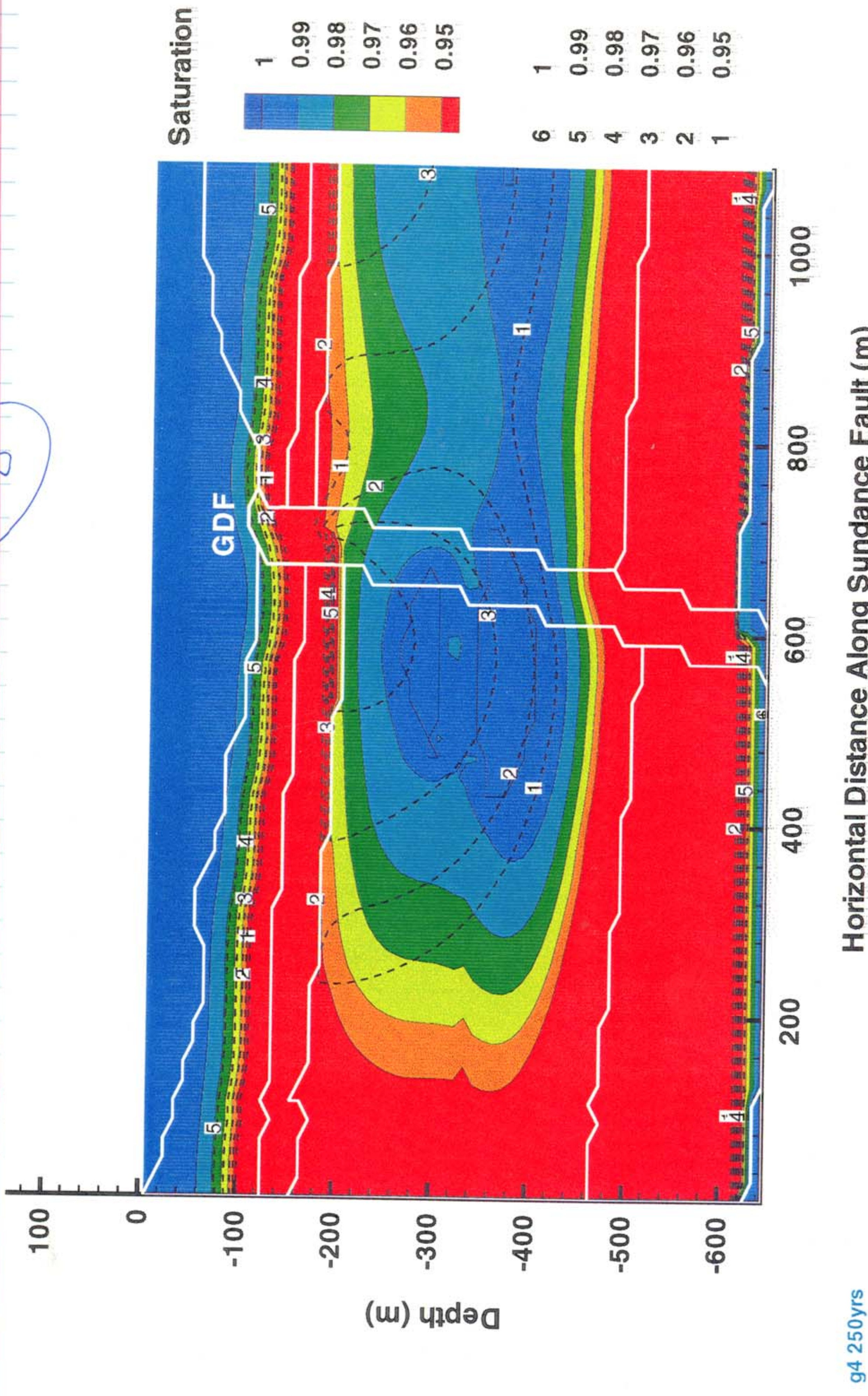


Figure on This Page

Same as on Page 20, except this page is for 250 yr following start of repository heating.



A complete time history of the perched water zone volume is shown in Figure 3 for three saturation thresholds (99.8, 99.98, and 100%). Several observations can be made from this figure. First, though the isothermal analyses produced high saturations, giving water volumes (per unit section thickness) of 4,800 and 7,500 m^3 within zones with saturations higher than 99.98 and 99.8%, respectively, there was no zone with saturation values equal to 100%. Under the influence of repository heating, the perched water volume based on 100% saturation threshold increases, reaches a maximum of 4,000 m^3 after 100 yrs and dissipates totally after 1,000 yrs. Similar behavior is exhibited by the other two curves with the exception of the maximum being attained around 45 yrs, followed by an abrupt decrease in the volume. The abrupt decrease in volume for both the 99.8 and 99.98% saturation values is attributed to condensation effects due to the heat wave reaching and passing through the area of isothermally-driven high saturation values.

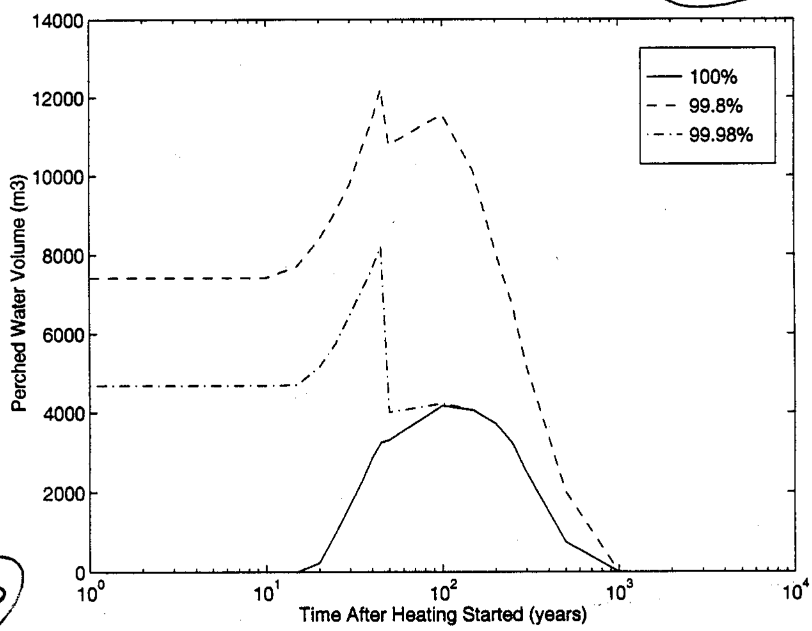


Figure 3. Time history of water volume for parts of the domain with saturations higher or equal to 99.8, 99.98 and 100%.

It is also worth reporting that even though the effects of repository heating are propagated and felt throughout the domain almost instantaneously, it takes a very long time for the system to return to its pre-heating state. A case in point is made by observing Figure 4, which depicts liquid-phase velocity magnitude contours and direction vectors after a period of 10,000 yrs. Comparing Figure 4 to Figure 1b one can readily infer that the flow system is still far from returning to its isothermal steady-state condition and that even after a period of 10,000 yrs.

Plots of gas-velocity magnitudes and directions (e.g., Figure 5a) were examined to understand the physical phenomena associated with the formation of perched water bodies under nonisothermal conditions in the vicinity of the repository. As Figure 5a shows, the introduction of heating caused general movement of gas away from the repository area, whereas water-movement directional patterns remained essentially the same as was established prior to repository heating. The combined effect of water accumulation and gas expulsion led to the development of 100%-saturation, first in the zone of highest isothermally-driven saturation. The size of the 100%-saturation zone initially increases with time and later migrates downwards to a depth of about 360-400 m, that is below the repository level (Figure 5b). Thereafter, the saturation zone begins to break up and eventually disappears, because of gas-driven moisture movement.

Figure on This Page

Liquid-phase velocity magnitude contours and direction vectors at 10,000 yrs after start of repository heating.

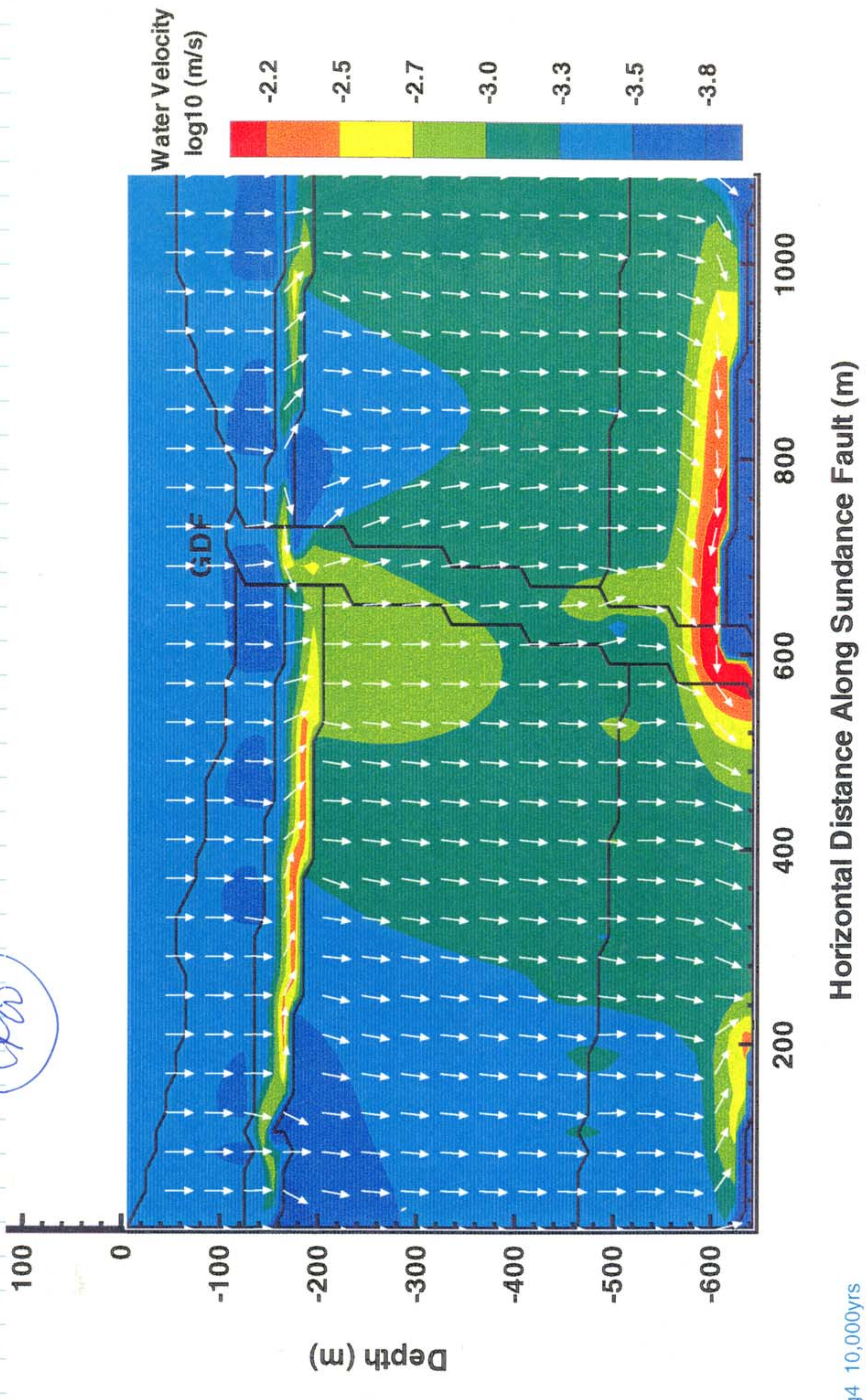
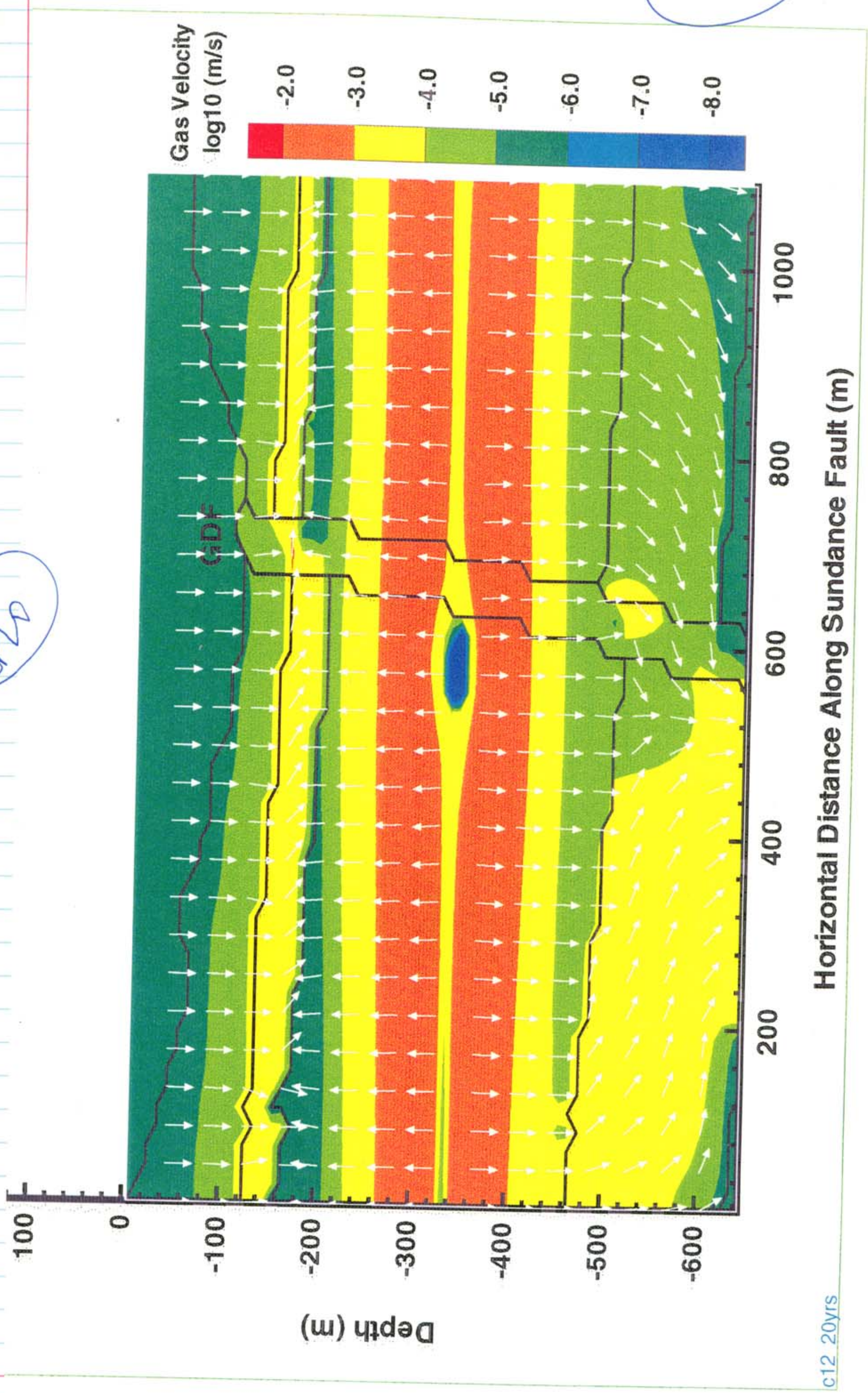


Figure on This Page

Gas-phase velocity magnitude contours and direction vectors at 20 yr following start of repository heating.

GW

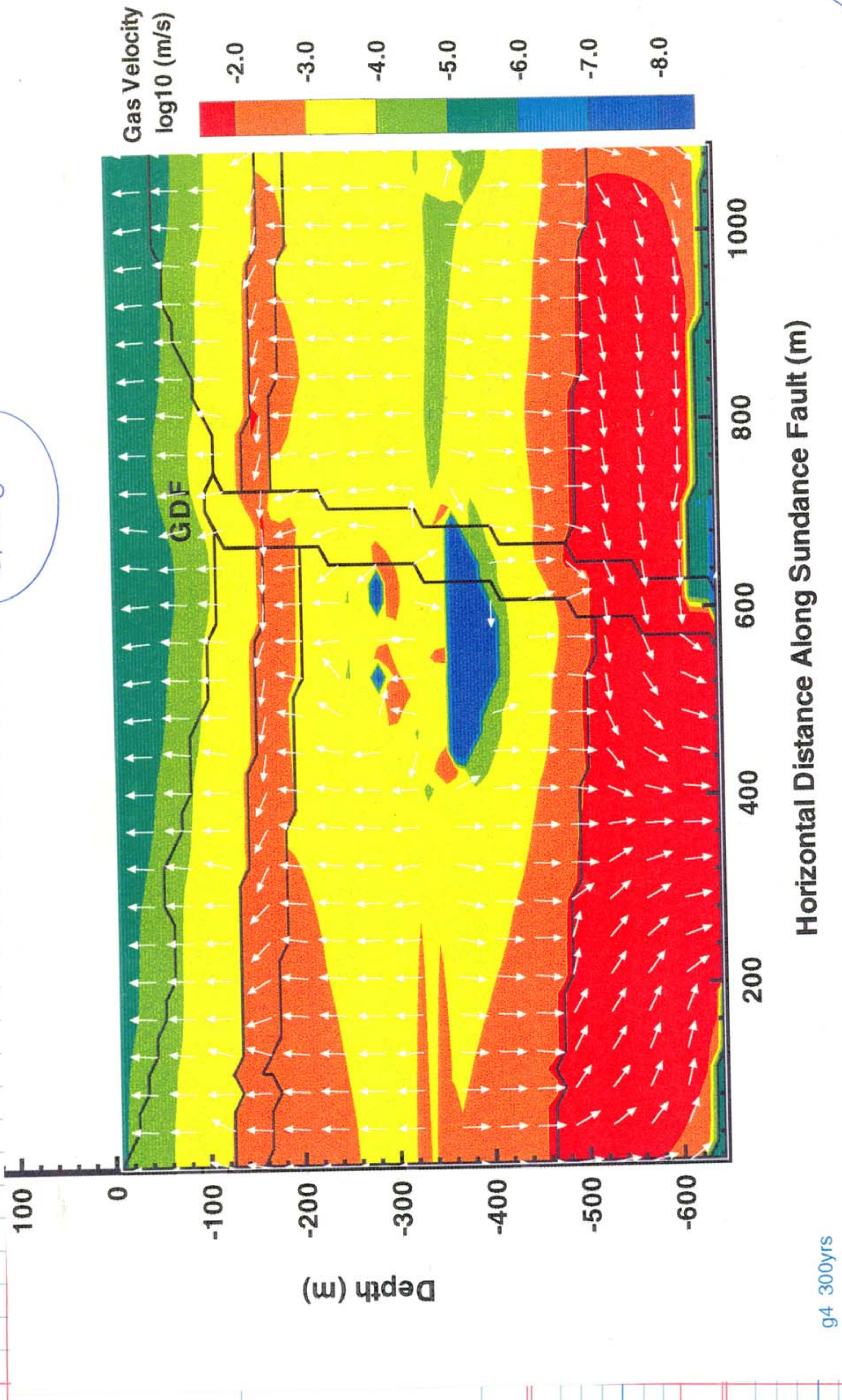


GW

~~Page~~ figure on This Page

Same as on p. 25, except that current figure is for 300 yr.

(GWD)



(GWD)

CONCLUSIONS

Results calculated so far in this work indicate that the initial effect of repository heating (under the condition of steady averaged infiltration) is likely to be increased water saturation within the repository area, because of gas expulsion from the heated area and water infiltration. Such increased saturation may result in sustained perched water volumes that grow in size within the first 100 yrs of repository heating and begin to dissipate thereafter.

Effect of Fractures — Sept 16 1996

The computer code METRA accounts for the hydrologic effects of fractures using the equivalent continuum model (ECM). The ECM replaces the permeability and porosity of the medium with bulk permeability k_b and bulk porosity ϕ_b, defined as follows:

$$\phi_b = \phi_f + (1 - \phi_f)\phi_m$$

$$k_b = k_m(1 - \phi_f) + k_f \phi_f$$

ϕ_m = matrix porosity
ϕ_f = fracture porosity
k_m = matrix permeability
k_f = fracture permeability

~~The~~ Matrix and fracture properties from TSPA-95 were used to implement an ECM model. The PCKR input block for the ECM cases is reproduced below:

```
PCKR
:   i  type-curv swirm  rpmm(lamda)  alpham    sgextm  sgc     iecm
:                swirf  rpmf(lamda)  alphaf    phim    phif    permm     permf
    1  Van-Gen   0.020  0.3582        8.4e-7   0.      0.      1
                 0.04   0.7636       1.305e-5  0.087   1.8e-3  9.7e-19   3.9e-12
    2  Van-Gen   0.100  0.8545       1.53e-6   0.      0.      1
                 0.040  0.7636       1.305e-5  0.421   1.8e-3  3.9e-14   3.9e-13
    3  Van-Gen   0.080  0.4438       5.8e-7    0.      0.      1
                 0.040  0.7636       1.305e-5  0.139   1.8e-3  1.9e-18   3.9e-12
    4  Van-Gen   0.041  0.741        1.63e-6   0.      0.      1
                 0.040  0.7636       1.305e-5  0.331   1.8e-3  2.7e-14   3.9e-13
    5  Van-Gen   0.110  0.3758       3.10e-7   0.      0.      1
                 0.040  0.7636       1.305e-5  0.306   1.8e-3  2.0e-18   3.9e-12
0
```

ECM Case 1

The input file (ecm1.dat) for ECM Case 1 isothermal analysis is shown below. The purpose of the isothermal analysis is to obtain the long-term (steady-state) water distribution prior to repository heating. The calculated results form the initial condition for the nonisothermal analysis. The infiltration rate and matrix properties are the same as applied in the cases described previously.

GO

Listing for Goodluck Ofoegbu

```
Example 2D Perched-Water Problem
Case ecm1: ECM equivalent of Case c08.
: Infiltration equal to TC Ksat(matrix); initial saturation of 25%
RSTART 0
:
: Grid definition
:
GRID XYZ 55 1 65 0 1 1
DXYZ 0
20.0
1.0
10.0
:
: Material-properties definition and assignment to grid blocks
:
THERM
: no rho        cpr    ckdry  cksat    crp  crt   tau   cdiff    cexp  enbd
   1  2.580e+03 840.0  1.74    2.3      0    0     .0   2.13e-5  1.8    1.
   2  2.580e+03 840.0  1.74    2.3      0    0     .0   2.13e-5  1.8    1.
   3  2.580e+03 840.0  1.74    2.3      0    0     .0   2.13e-5  1.8    1.
   4  2.580e+03 840.0  1.74    2.3      0    0     .0   2.13e-5  1.8    1.
   5  2.580e+03 840.0  1.74    2.3      0    0     .0   2.13e-5  1.8    1.
0
PCKR
:   i  type-curv swirm  rpmm(lamda)  alpham    sgextm  sgc     iecm
:                swirf  rpmf(lamda)  alphaf    phim    phif    permm      permf
    1  Van-Gen   0.020  0.3582         8.4e-7  0.      0.      1
                 0.04   0.7636       1.305e-5  0.087   1.8e-3  9.7e-19    3.9e-12
    2  Van-Gen   0.100  0.8545       1.53e-6   0.      0.      1
                 0.040  0.7636       1.305e-5  0.421   1.8e-3  3.9e-14    3.9e-13
    3  Van-Gen   0.080  0.4438       5.8e-7    0.      0.      1
                 0.040  0.7636       1.305e-5  0.139   1.8e-3  1.9e-18    3.9e-12
    4  Van-Gen   0.041  0.741        1.63e-6   0.      0.      1
                 0.040  0.7636       1.305e-5  0.331   1.8e-3  2.7e-14    3.9e-13
    5  Van-Gen   0.110  0.3758       3.10e-7   0.      0.      1
                 0.040  0.7636       1.305e-5  0.306   1.8e-3  2.0e-18    3.9e-12
0
PHIK  ec01          : Get material assignments from ec01.phk
:
: Initial conditions
:
INIT
    1   55    1    1     1   64   1.0725e+05    25.000   0.75      0   0
    1   55    1    1    65   65   1.0725e+05    25.000   0.0001   0   0
0
RECUrrent-data
:
OUTPUT P=1 L=1 T=1
SOLVE   4   2   7
:
:TOLR TOLP  TOLS  TOLT  TOLP2  TOLM  TOLA  TOLE
Tolr  1.e-0 1.e-4 1.e-3 1.e+0  1.e-6 1.e-6 1.e-6 1.e-12  1.e-12  1.e-12
:
:Limit dpmx dsmx dtmpmx dp2mx dtmn    dtmx icutmx
LIMIT  5.e6 .07    7.    5.e6  1.e-8   1.e3  0
:
:AUTO-step  DPMXE    DSMXE DTMPMXE DP2MXe TACCEL IAUTO
AUTO-step   1.0E+5   0.03   3.0   1.e5
Plots 1
:
: Boundary conditions
:
BCON 2
  1 BOTTOM 1 55 1 1
  0   0  1.0725E5 25.0 0.0001 0
0
  3 TOP     1 55 1 1
  0   3.059E-4 1.0 25 0.0001 0
0
RSTART 1
:
STEADY[y] 1.E-4
ENDS
```

GO

The input file (ecn1.dat) for the nonisothermal case is shown on the next page. Both ecm1 and ecn1 require the following auxilliary input files:

GWO

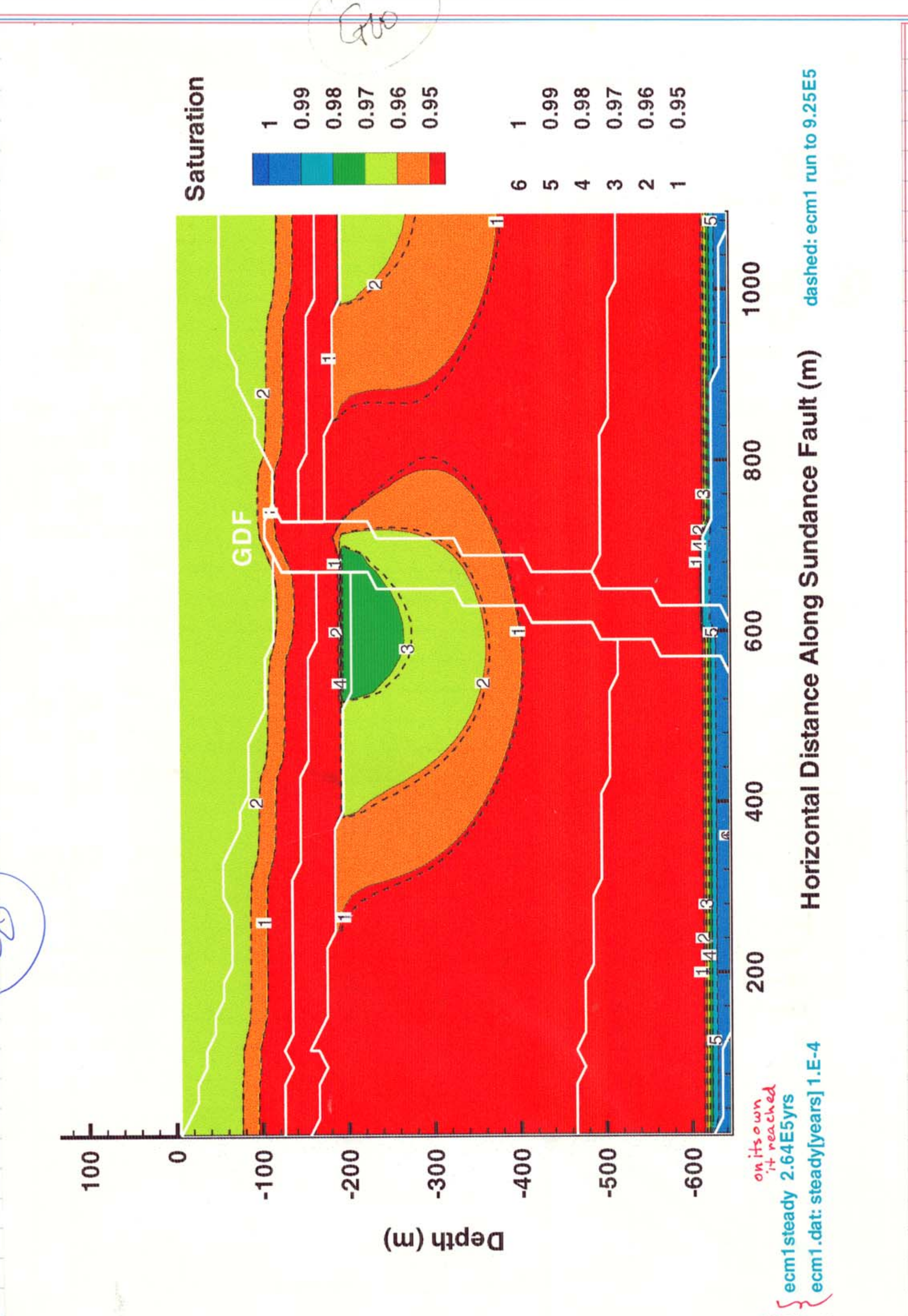
Listing for Goodluck Ofoegbu

```
Example 2D Perched-Water Problem
Case ecn1: Nonisothermal case; ecm1 steady state as initial condition
: Infiltration equal to TC Ksat(matrix); initial saturation of 25%
RSTART 0
:
: Grid definition
:
GRID XYZ 55 1 65 0 1 1
DXYZ 0
20.0
1.0
10.0
:
: Material-properties definition and assignment to grid blocks
:
THERM
: no rho        cpr    ckdry  cksat    crp  crt   tau  cdiff    cexp  enbd
   1  2.580e+03 840.0  1.74    2.3     0    0     .0  2.13e-5  1.8    1.
   2  2.580e+03 840.0  1.74    2.3     0    0     .0  2.13e-5  1.8    1.
   3  2.580e+03 840.0  1.74    2.3     0    0     .0  2.13e-5  1.8    1.
   4  2.580e+03 840.0  1.74    2.3     0    0     .0  2.13e-5  1.8    1.
   5  2.580e+03 840.0  1.74    2.3     0    0     .0  2.13e-5  1.8    1.
0
PCKR
:   i  type-curv swirm  rpmm(lamda)  alpham    sgextm  sgc     iecm
:                swirf  rpmf(lamda)  alphaf    phim    phif    permm      permf
    1  Van-Gen   0.020  0.3582         8.4e-7  0.      0.      1
                 0.04   0.7636       1.305e-5  0.087   1.8e-3  9.7e-19    3.9e-12
    2  Van-Gen   0.100  0.8545       1.53e-6   0.      0.      1
                 0.040  0.7636       1.305e-5  0.421   1.8e-3  3.9e-14    3.9e-13
    3  Van-Gen   0.080  0.4438       5.8e-7    0.      0.      1
                 0.040  0.7636       1.305e-5  0.139   1.8e-3  1.9e-18    3.9e-12
    4  Van-Gen   0.041  0.741        1.63e-6   0.      0.      1
                 0.040  0.7636       1.305e-5  0.331   1.8e-3  2.7e-14    3.9e-13
    5  Van-Gen   0.110  0.3758       3.10e-7   0.      0.      1
                 0.040  0.7636       1.305e-5  0.306   1.8e-3  2.0e-18    3.9e-12
0
PHIK  ec01          : Get material assignments from ec01.phk
:
: Initial conditions
:
INIT ecm1ss         : Get initial condition from ecm1ss.int
:
RECUrrent-data
:
OUTPUT P=1 L=1 T=1
SOLVE   4   2   7
:
:TOLR TOLP  TOLS  TOLT  TOLP2  TOLM  TOLA  TOLE
Tolr  1.e-0 1.e-4 1.e-3 1.e+0  1.e-6 1.e-6 1.e-6 1.e-12  1.e-12  1.e-12
:
:Limit dpmx dsmx dtmpmx dp2mx dtmn     dtmx icutmx
LIMIT  5.e6 .07    7.    5.e6  1.e-8    1.e3  0
:
:AUTO-step  DPMXE    DSMXE DTMPMXE DP2MXe TACCEL IAUTO
AUTO-step   1.0E+5   0.03   3.0    1.e5
Plots 1
SOURCE  1  1.0  1.0  qh83   : read heat source definition from qh83.src
:
: Boundary conditions
:
BCON 2
  1 BOTTOM 1 55 1 1
  0    0  1.0725E5 25.0 0.0001 0
0
  3 TOP    1 55 1 1
  0    3.059E-4 1.0 25 0.0001 0
0
:RSTART 1
:
TIME[years] 1
TIME[years] 5
TIME[years] 10
TIME[years] 15
TIME[years] 20
TIME[years] 40
TIME[years] 50
TIME[years] 100
TIME[years] 200
TIME[years] 300
TIME[years] 500
TIME[years] 5000
TIME[years] 10000
ENDS
```

GWO

ec01.phk	Material-index assignment. Required by both ecm1 and ecn1.
ecm1ss.int	Initial conditions based on ecm1 steady-state solution. Required by ecn1 only
qh83.src	Heat-source definition. Required by ecn1 only.

Results are presented on the following pages.



Steady-State saturation for ecm1 case.
Two sets of results presented confirm that the solution is satisfactorily close to steady state.

The steady-state solution on Page 30 compare with the matrix-flow-only case (Page 17) as follows:

(1) The shape of the high-saturation zone is essentially the same in both cases. ~~es~~ (GW)

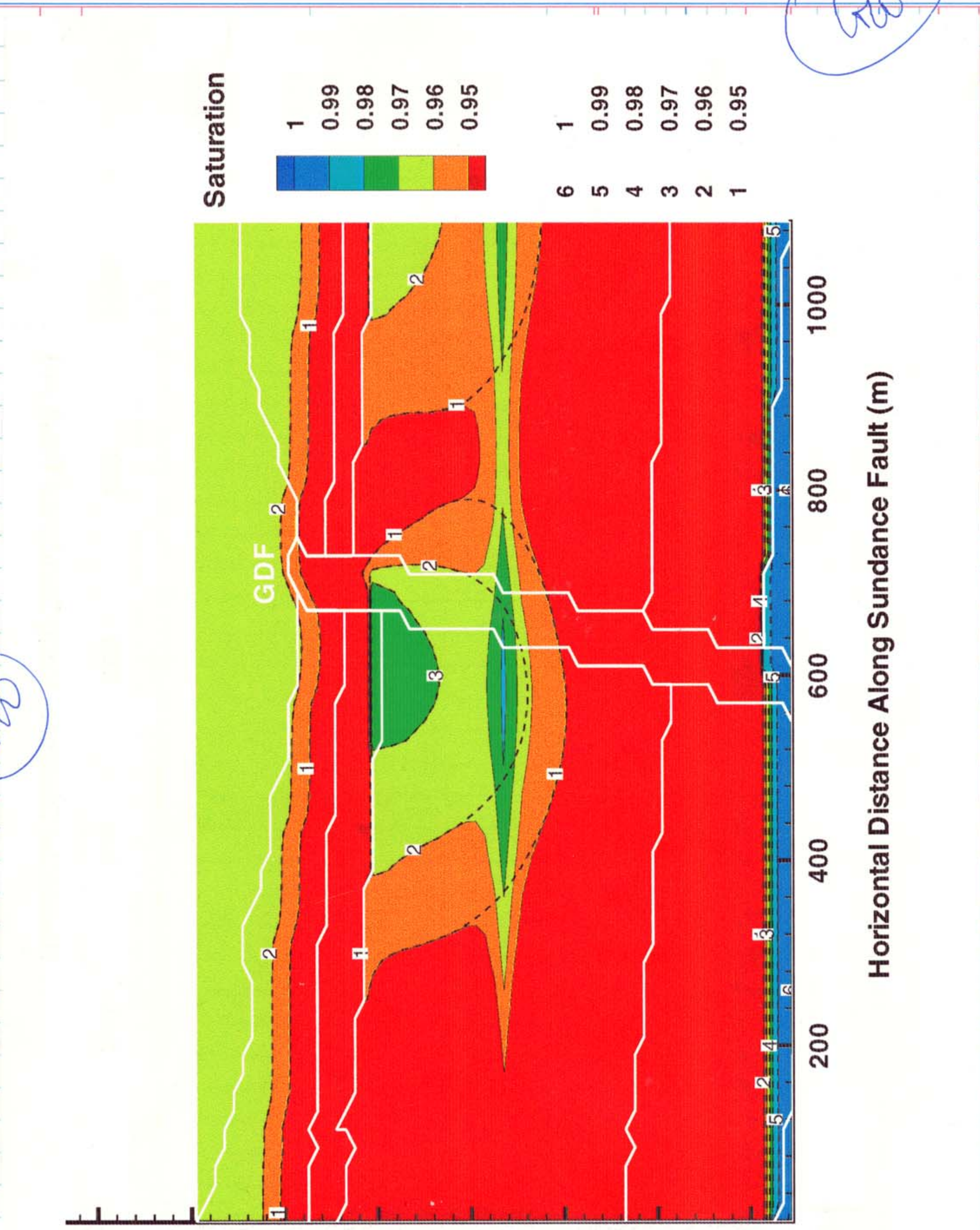
(2) The highest steady-state saturation falls in the range 0.98 – 0.99 in the matrix-flow case, but in 0.97 – 0.98 for the ECM case.

It should be noted that the infiltration rate applied in both analyses (~ 0.3 mm/yr) is equal ~~to the hydraulic conductivity of the top layer~~ (GW) to the saturated hydraulic conductivity of the top layer (TC member) in the matrix-flow case but much less in the ECM case

Case	K_{sat} of top layer	Applied infiltration
Matrix flow	9.7×10^{-12} m/s	3.059×10^{-4} m/yr $= 9.7 \times 10^{-12}$ m/s
ECM	7.02×10^{-8} m/s	Same.

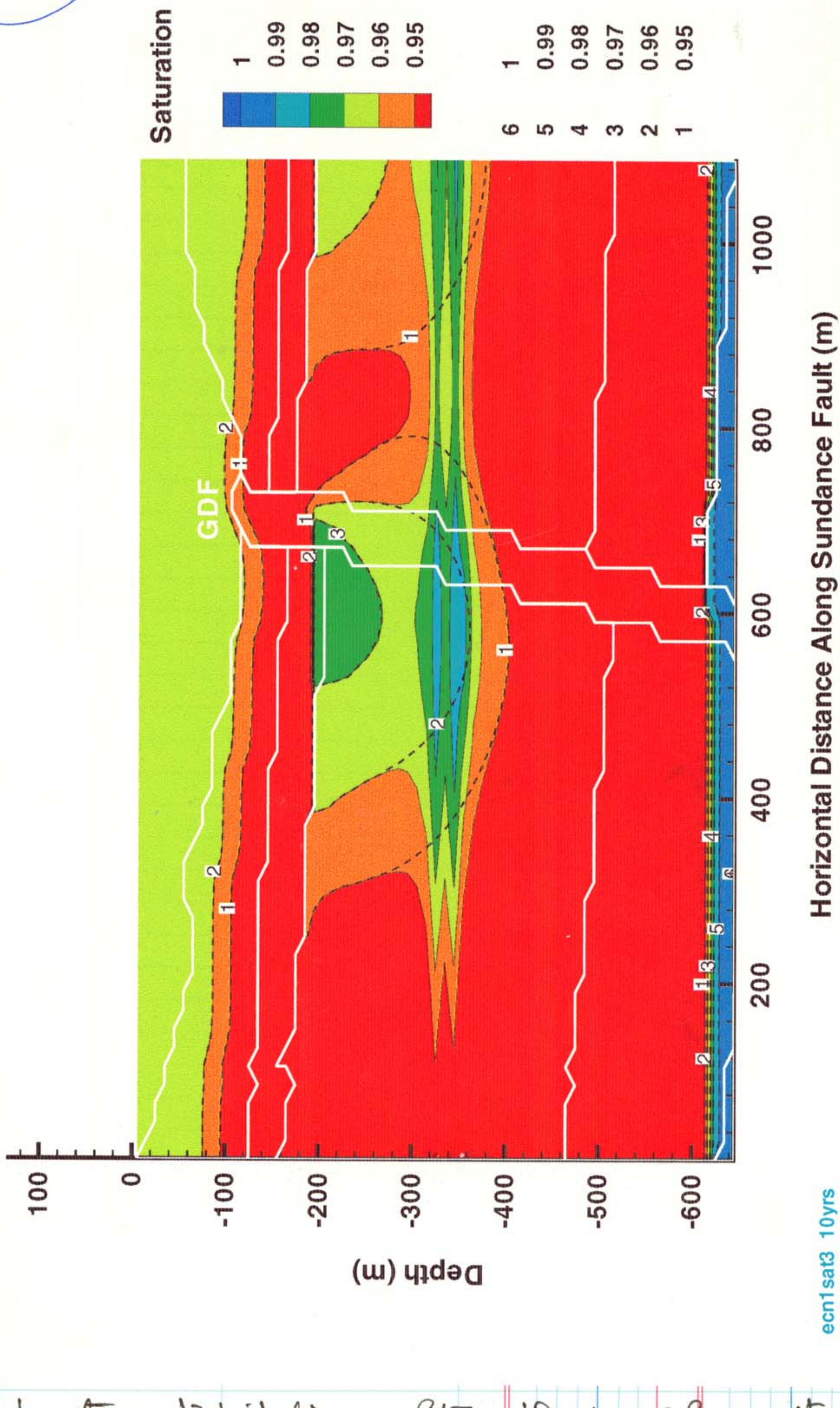
It will be necessary to rerun the ECM case with higher infiltration in order to assess the perched-water potential properly. But first, the nonisothermal results from ecn1 (nonisothermal analysis with ecm1 steady state as initial condition) are presented.

GEO



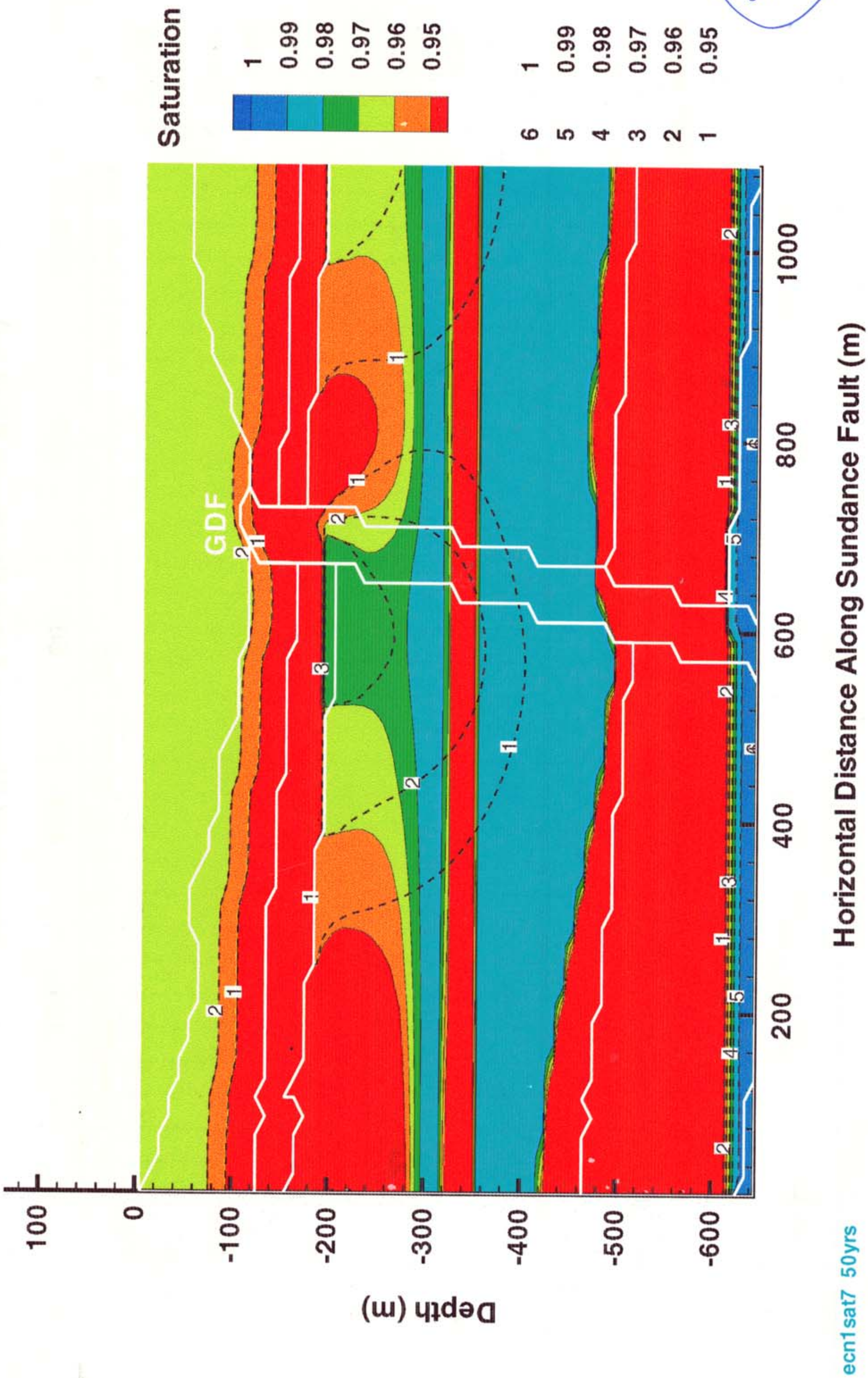
Saturation distribution after 5 yrs of repository heating. Dashed lines are the steady-state isothermal solution.

GW

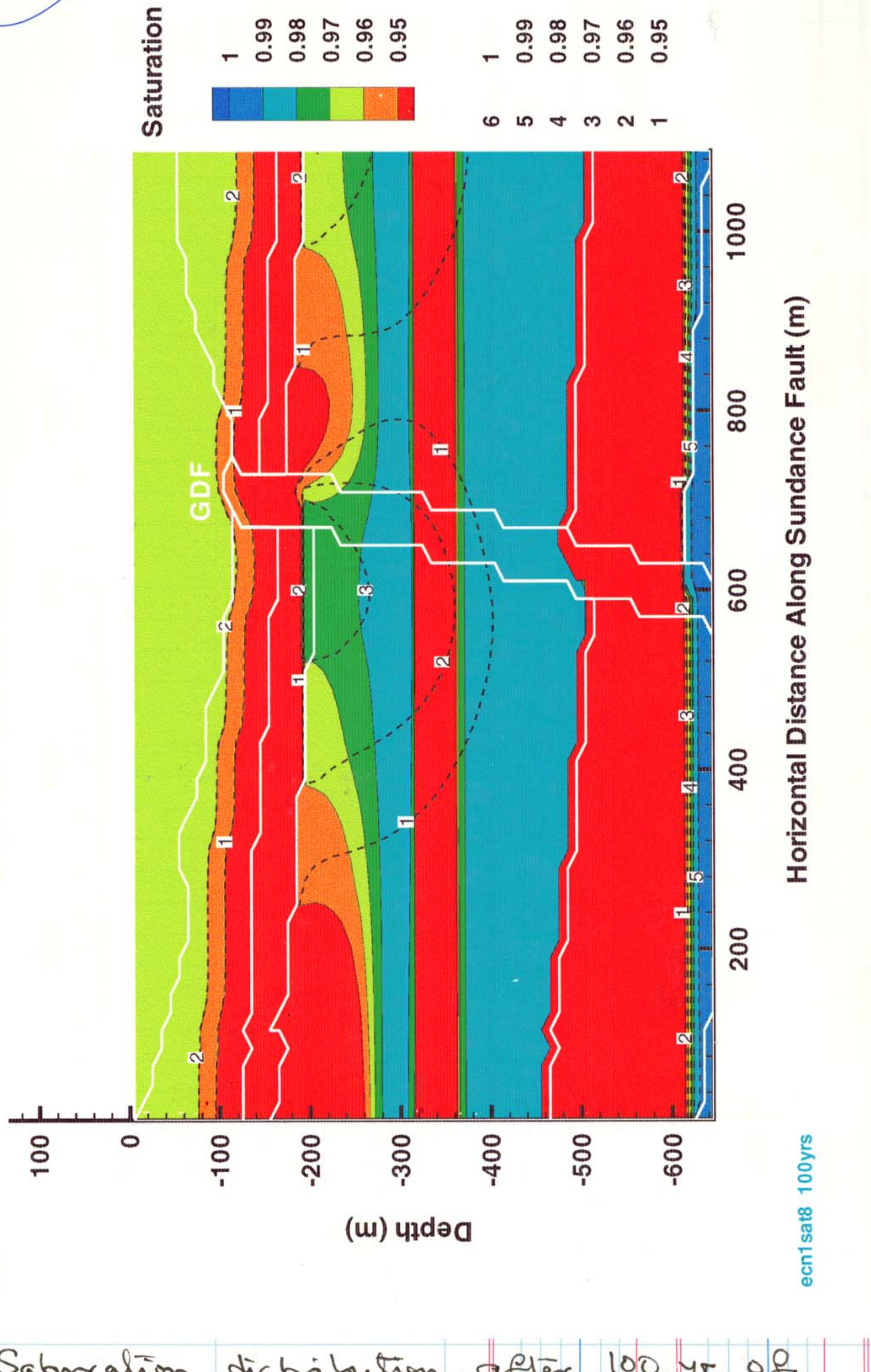


GW

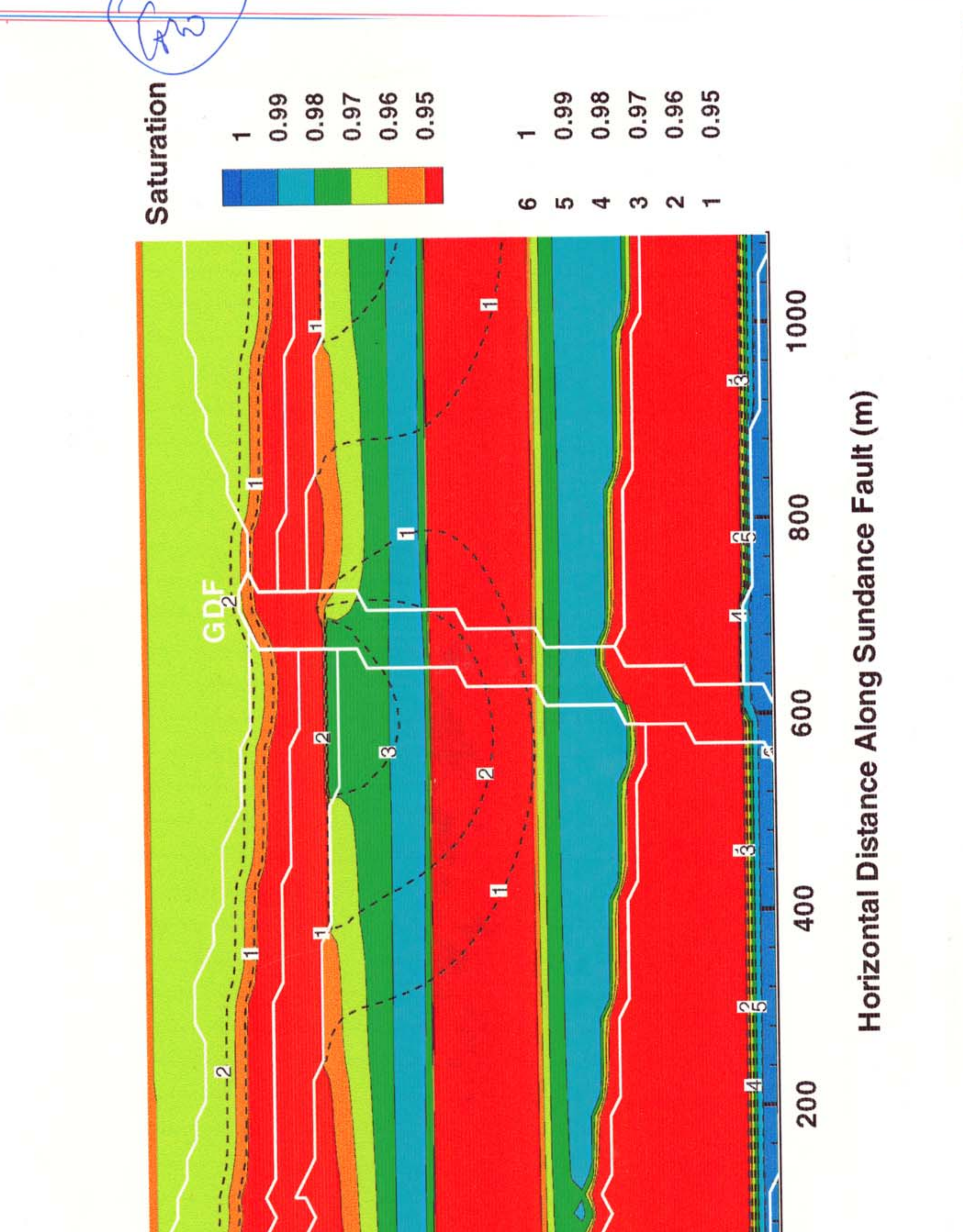
Saturation distribution after 10 yrs of repository heating. Dashed lines represent steady-state isothermal solution.



Saturation distribution after 50 yr of repository heating. Dashed lines represent steady-state isothermal solution.



Saturation distribution after 100 yr of repository heating. Dashed lines represent steady-state isothermal solution.



Saturation distribution after 500 yr of repository heating. Dashed lines represent steady state isothermal solution.

November 2 1996

ECM Cases with Higher-Infiltration Rates

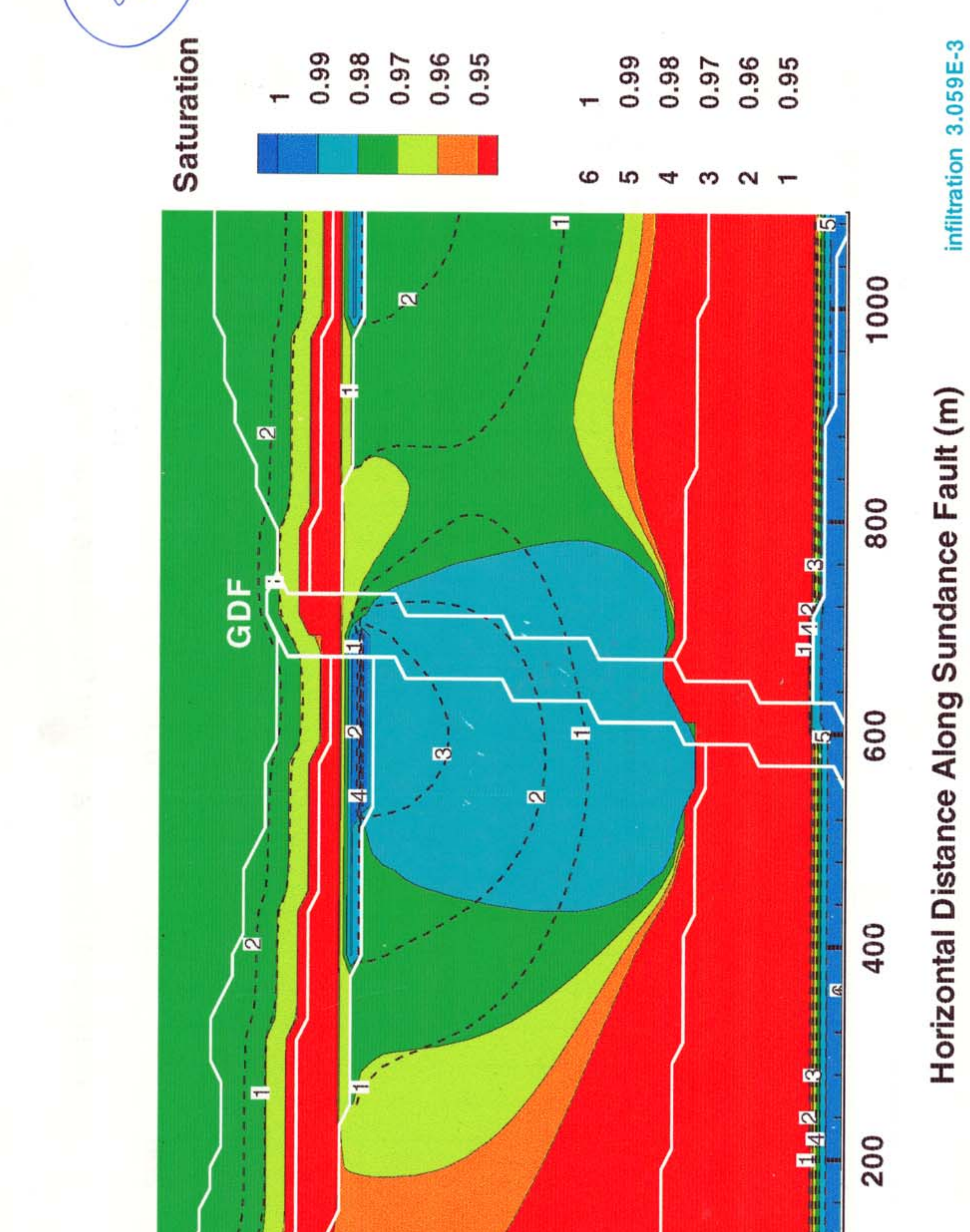
~~The~~ Two additional ECM cases were run, with the material properties given on page 27. The infiltration rates applied in these cases are as follows:

ECM2	Isothermal	3.059 mm/yr
ECN2	Nonisothermal	3.059 mm/yr
ECM3	Isothermal	30.59 mm/yr
ECN3	Nonisothermal	30.59 mm/yr

As was done previously, each analysis case consists of an isothermal analysis step to steady state followed by a nonisothermal analysis step to 10000 yrs beyond the end of the isothermal analysis. Solution from the isothermal analysis was used as initial state for the nonisothermal analysis. Repository heating was simulated ~~using~~ (in the nonisothermal analysis) using the heat-source history defined in file qh83.src.

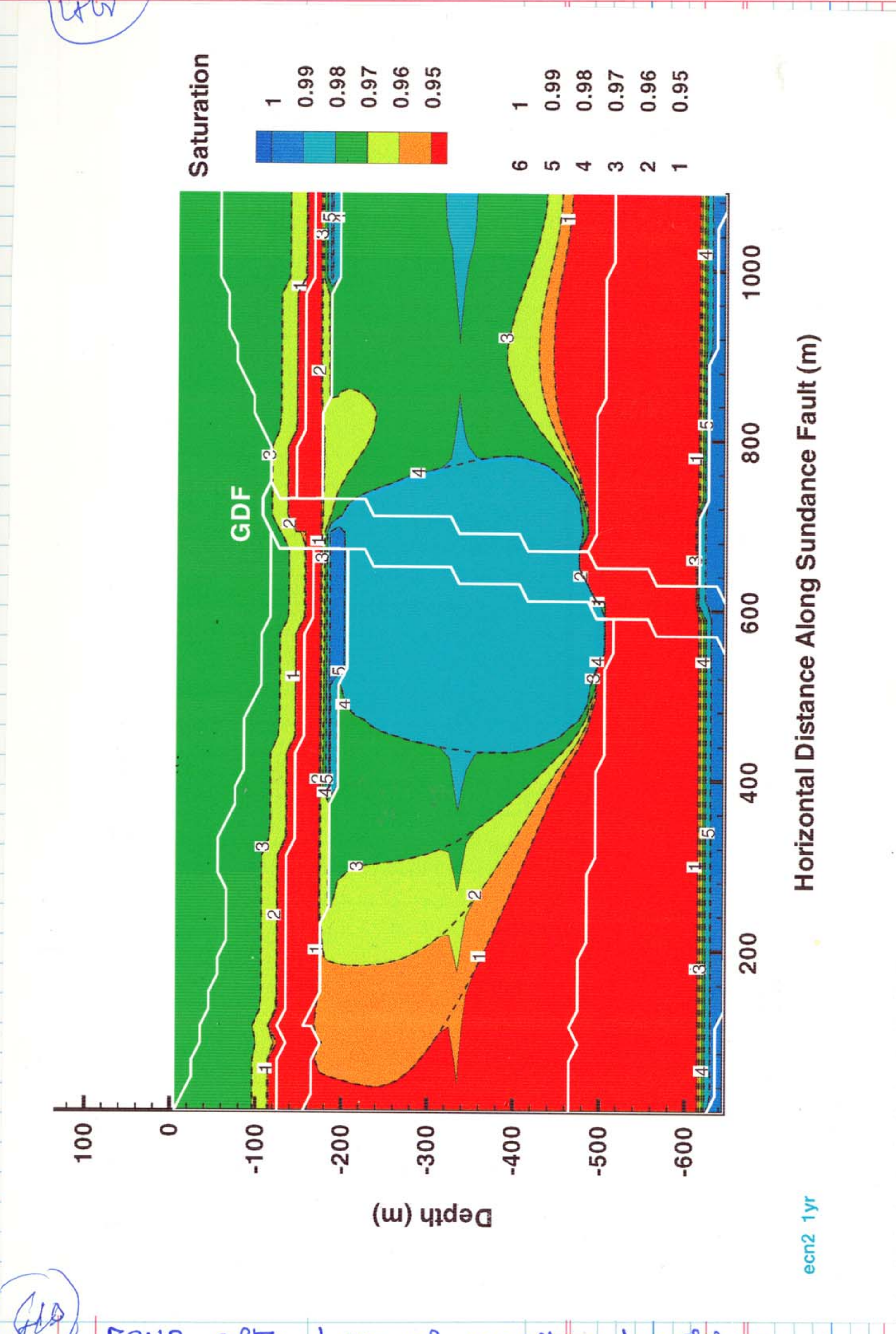
The results are presented in the following pages.

GWD

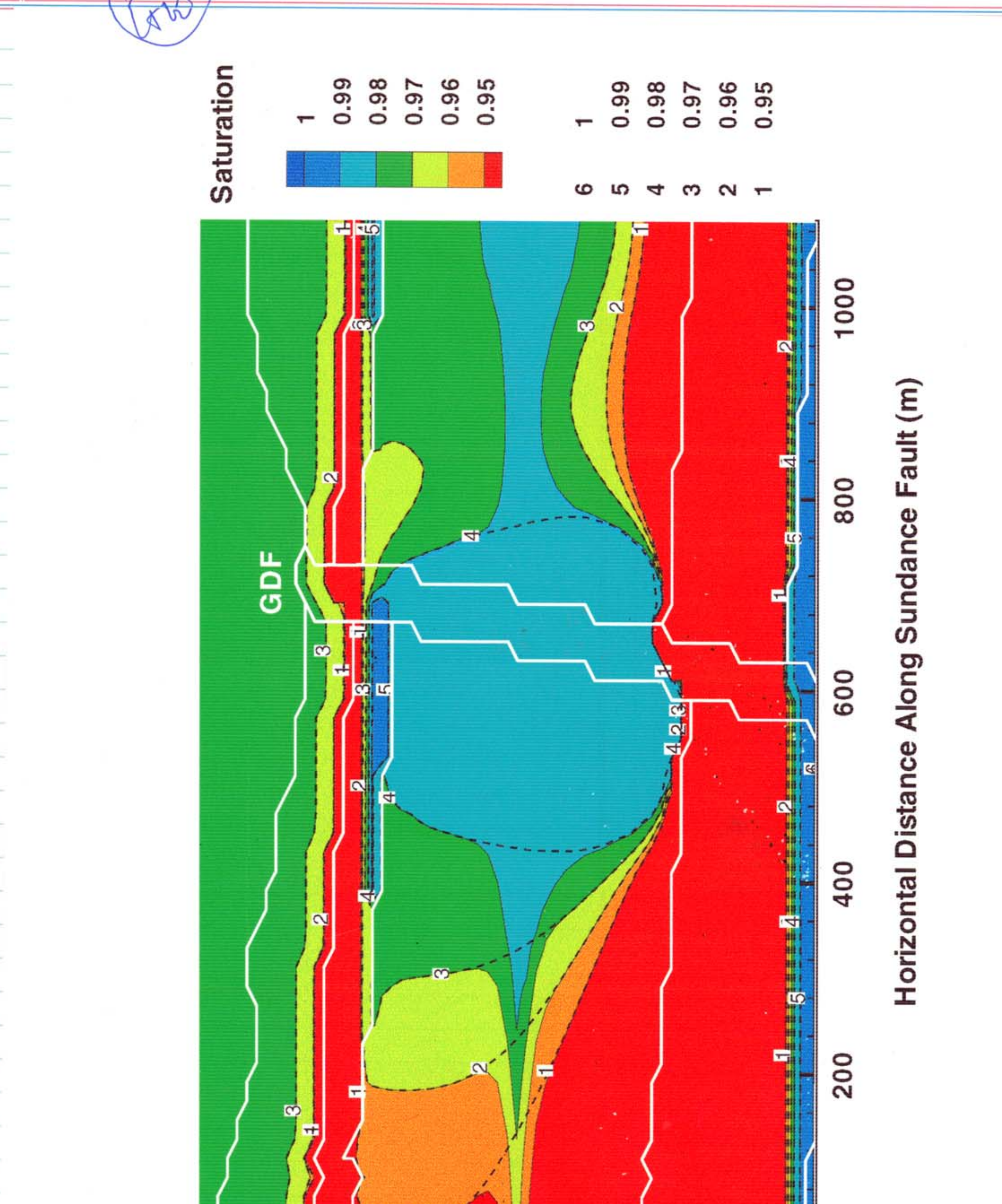


GWD

ECM2 Steady-State (isothermal case)
Infiltration rate: 3.059 mm/yr
Dashed lines represent steady-state solution for
GWD ~~matrix flow case: ecm1.sto case~~ GWD
ecm1 case (0.3 mm/yr)

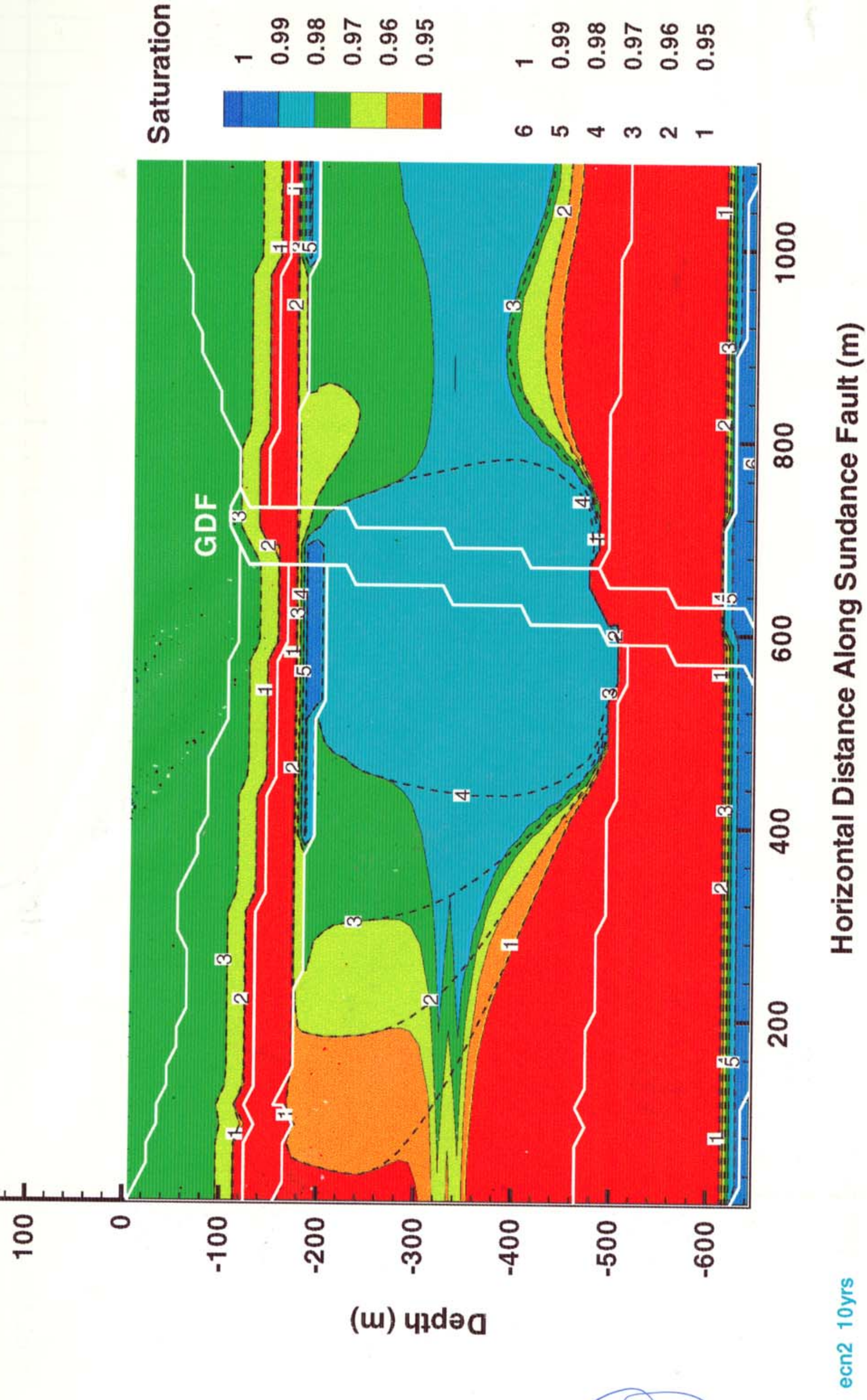


ECN2 after 1 yr of repository heating.
Infiltration rate: 3.059 mm/yr
Dashed lines represent isothermal steady-state solution.



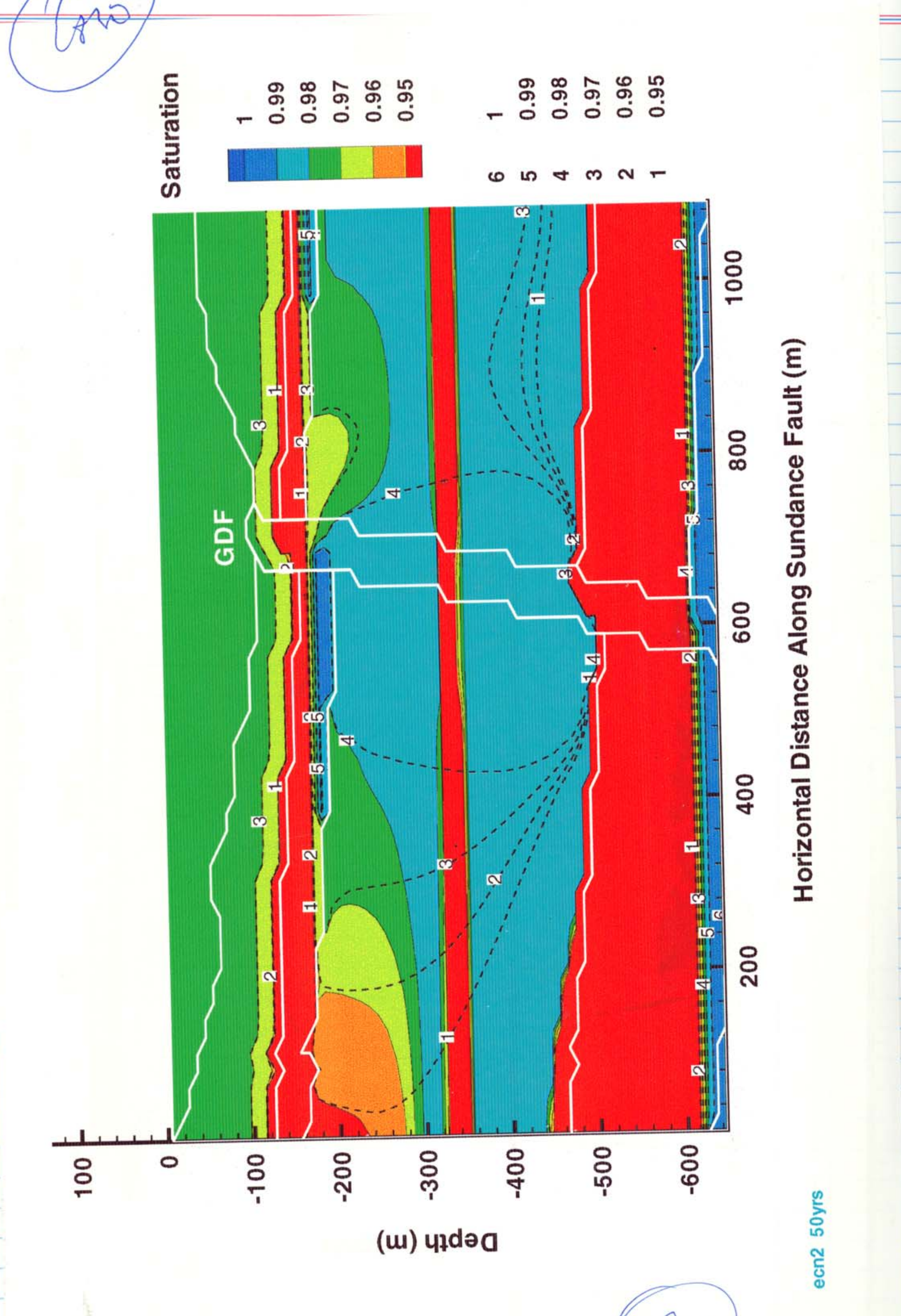
ECN2 after 5 yrs
Infiltration rate: 3.059 mm/yr
Dashed lines: Isothermal steady-state solution

(G10)

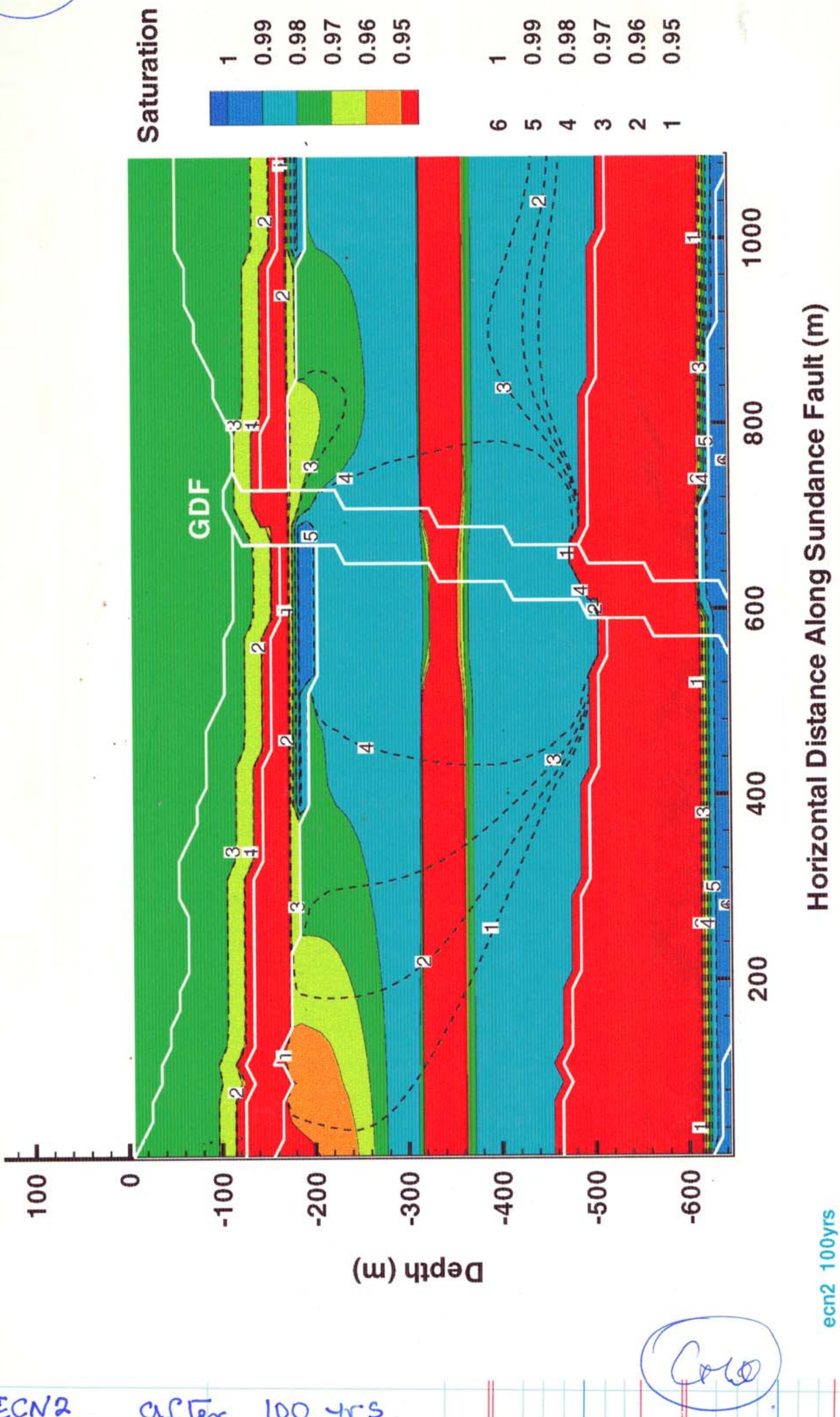


(G10)

ECN2 ~~X~~ after 10 yrs
Infiltration rate: 3.059 mm/yr
Dashed lines: Isothermal steady-state solution.

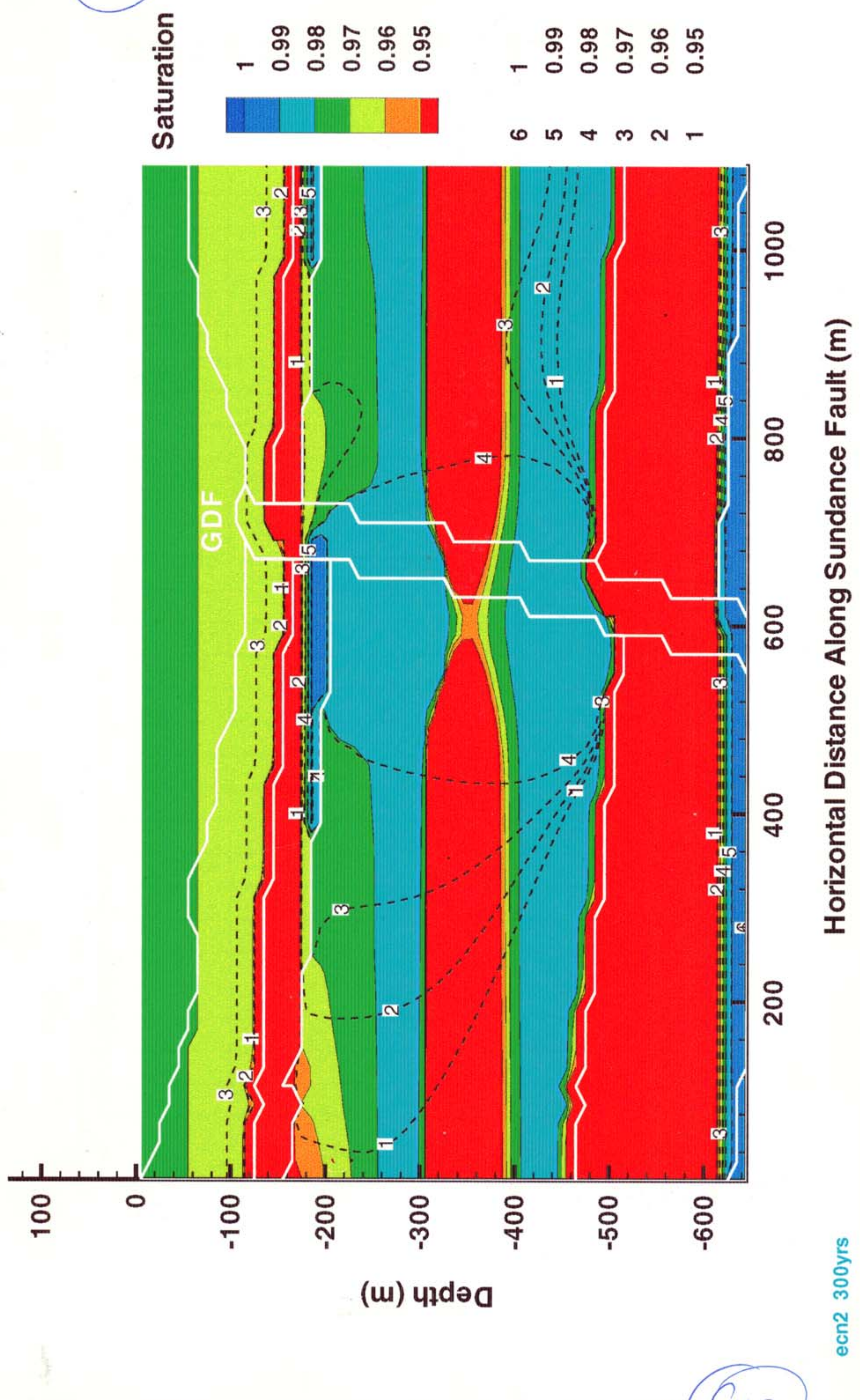


ECN2 after 50yrs
Infiltration rate: 3.059 mm/yr
Dashed lines: Isothermal steady-state solution



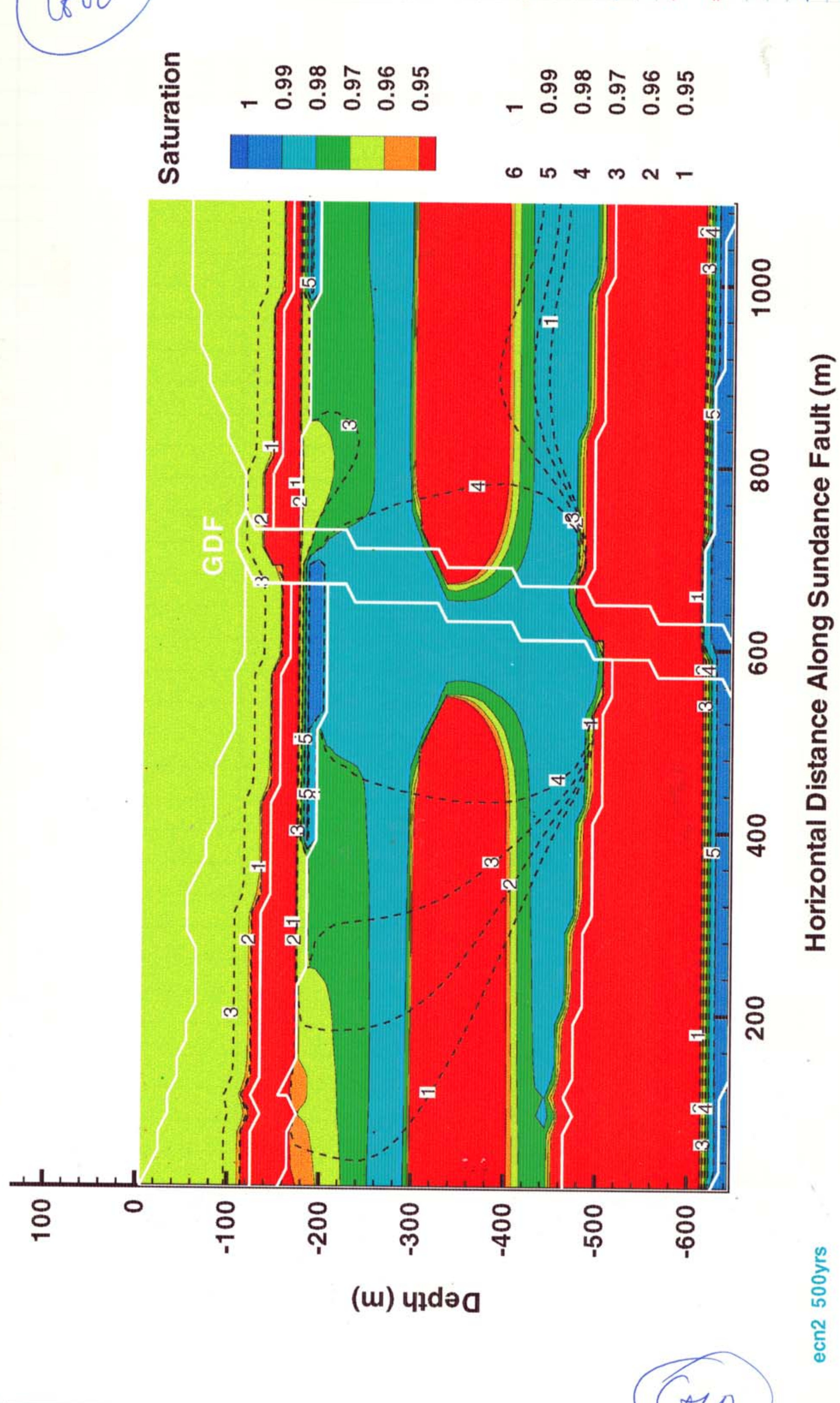
ECN2 after 100 yrs
Infiltration rate: 3.059 mm/yr
Dashed lines: Isothermal steady-state solution

Coro

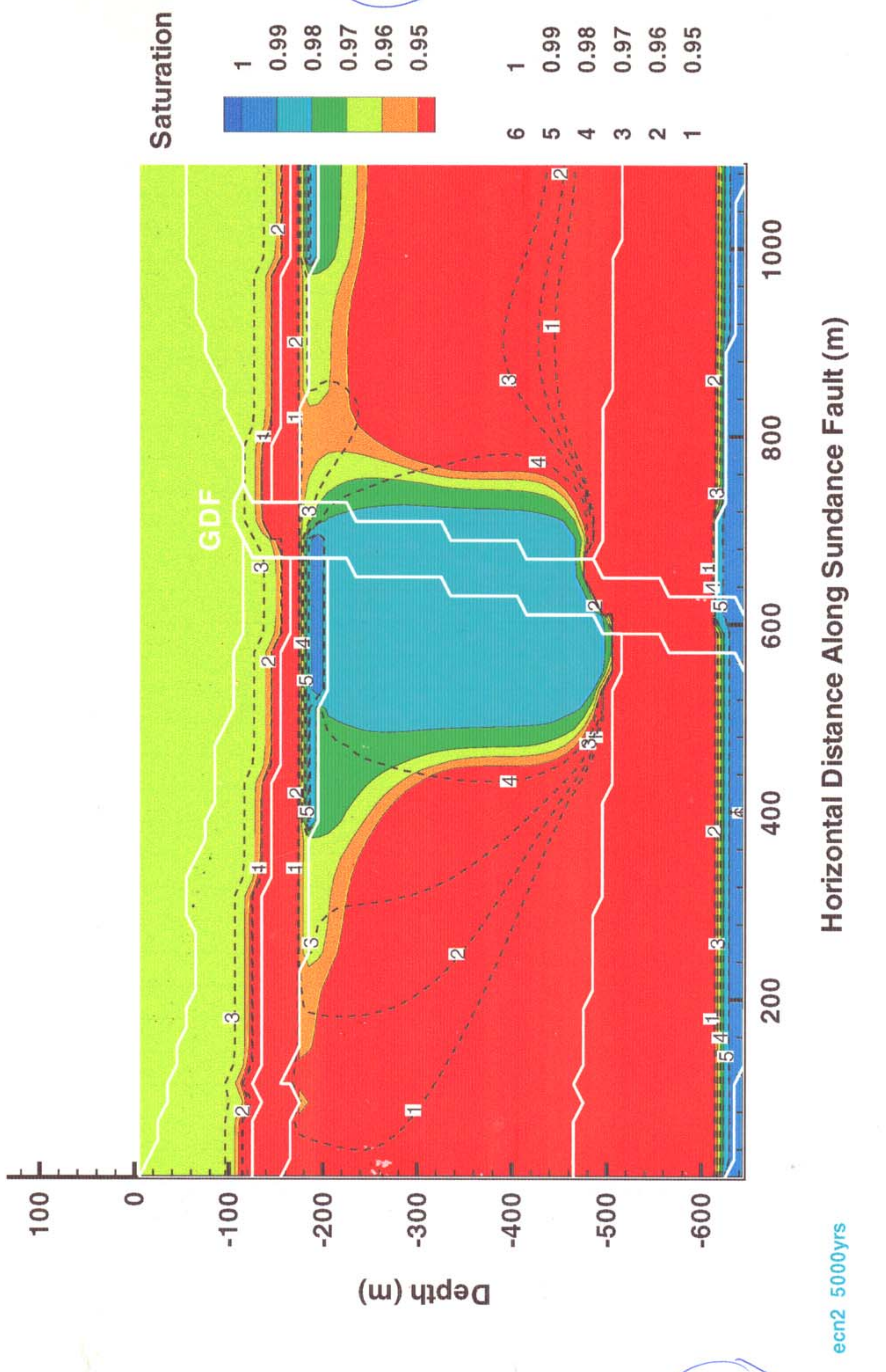


Coro

~~EN~~ ECN2 after 300 yrs
Infiltration rate: 3.059 mm/yr
Dashed lines: Isothermal steady-state solution

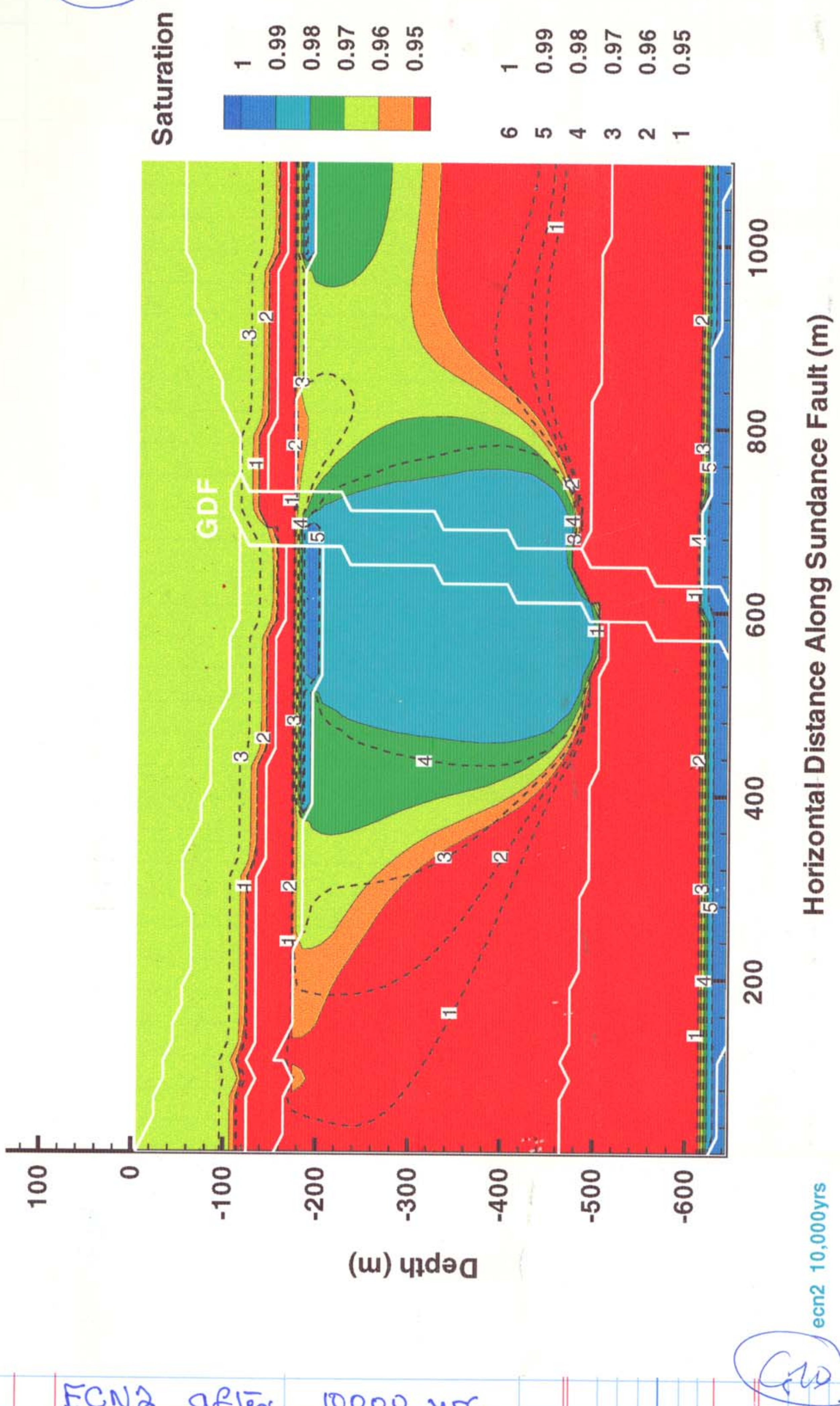


ECN2 after 500 yrs
Infiltration rate: 3.059 mm/yr
Dashed lines: Isothermal steady-state solution.



ECN2 after 5000 yrs
Infiltration rate: 3.059 mm/yr
Dashed lines: Isothermal steady-state solution

(G10)



(G10)

ECN2 after 10000 yrs
Infiltration rate: 3.059 mm/yr
Dashed lines: Isothermal steady-state solution

The results of ECM1 and ECN2 (isothermal and nonisothermal analyses, respectively, for infiltration rate of 3.059 mm/yr, with ECM model), presented on pages 38-47, show the following features:

(1) The isothermal steady-state solution includes two perched-water bodies; one in the PTn and the other in the TSw unit. The PTn perched body is smaller than the TSw perched body. The PTn perched body has saturations of 0.99-1.0 with positive pressure head ~~at some~~ within the middle. The TSw perched body has saturations of 0.98-0.99.

(2) At the introduction of repository heating both the ~~extent and do~~ spatial extent and degree of saturation within the TSw perched body increased. The increase in saturation occurred first at the repository horizon and spread vertically downward and upward away from the repository.

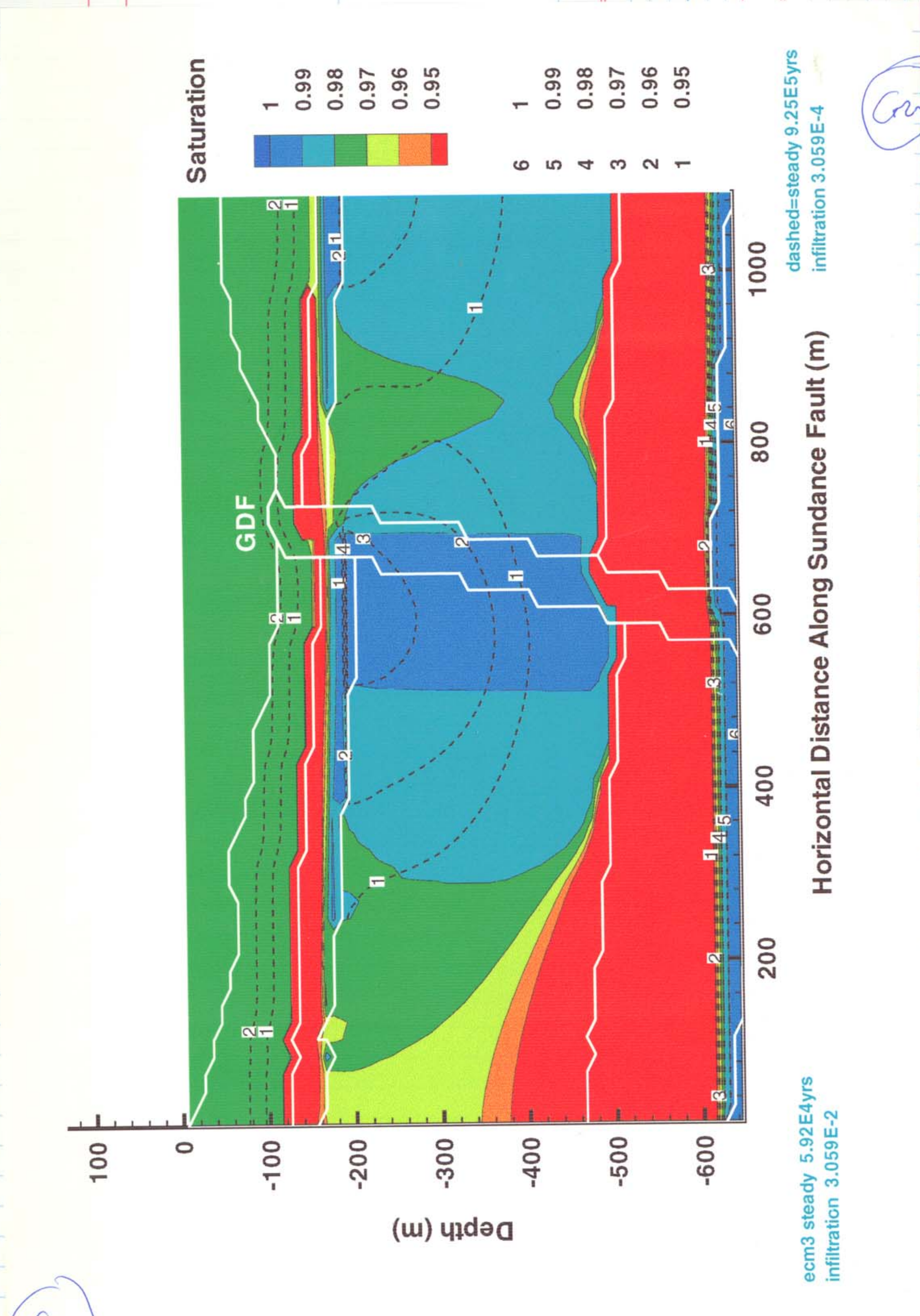
Drying (decrease in saturation) started at the repository horizon at about 10 yrs following heat introduction. The dry-out zone grew upward and downward up to about 300 yrs, when rewetting of the repository began. The saturation distribution at 10,000 yrs is almost back to the steady-state solution.

(3) The perched-water body in the PTn unit remained essentially unchanged throughout the 10,000-yr heating history.

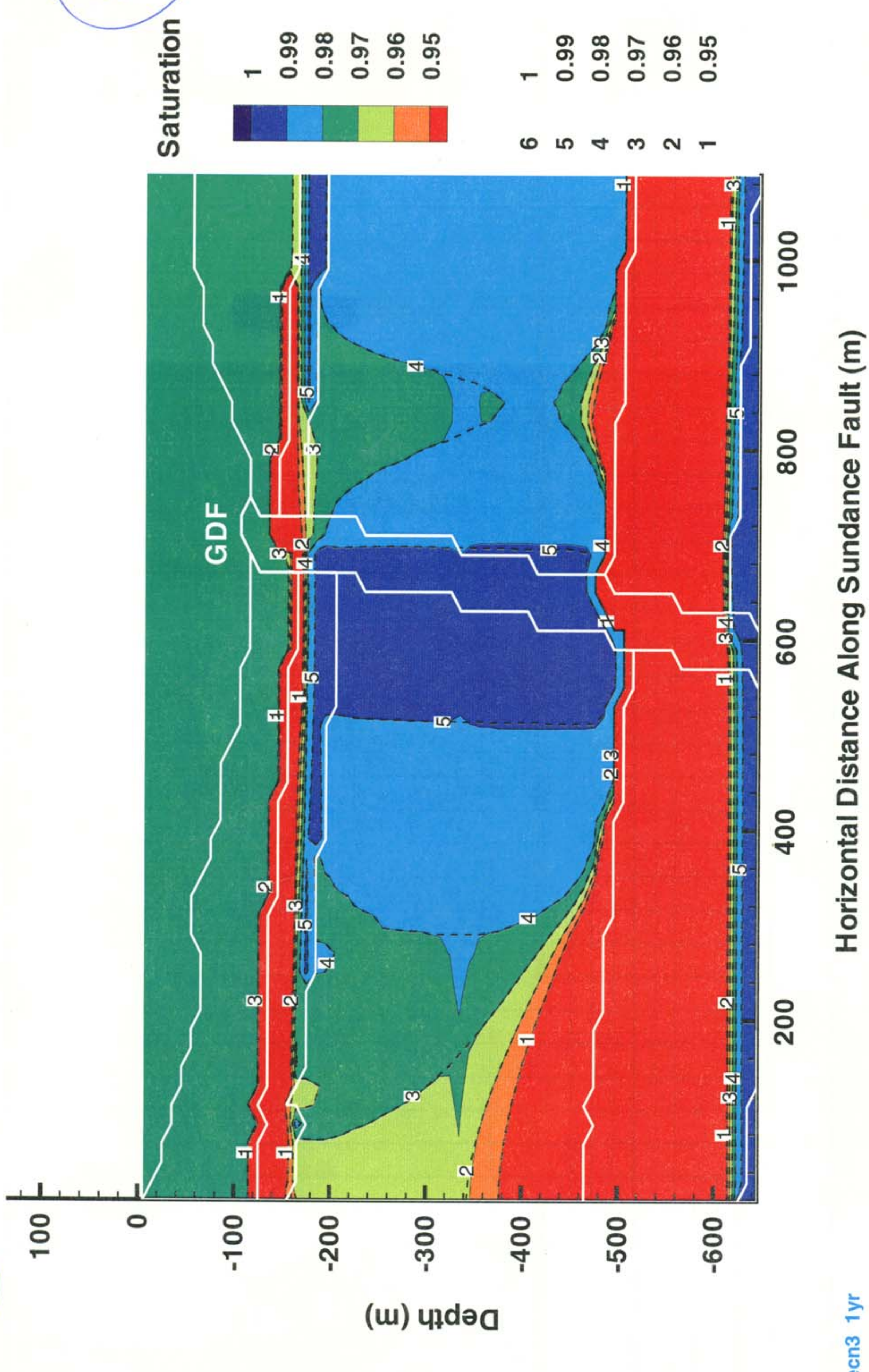
I have reviewed this part of this Scientific Notebook (pages 1-48) and find it in compliance with QAP-001 and there is sufficient technical information so that another qualified individual could repeat the activity

(A.H. Chowdhury)
Element Manager-RDCO
1-13-97

Jan 17 1997 ECN3 and ECM3 (See p. 37)



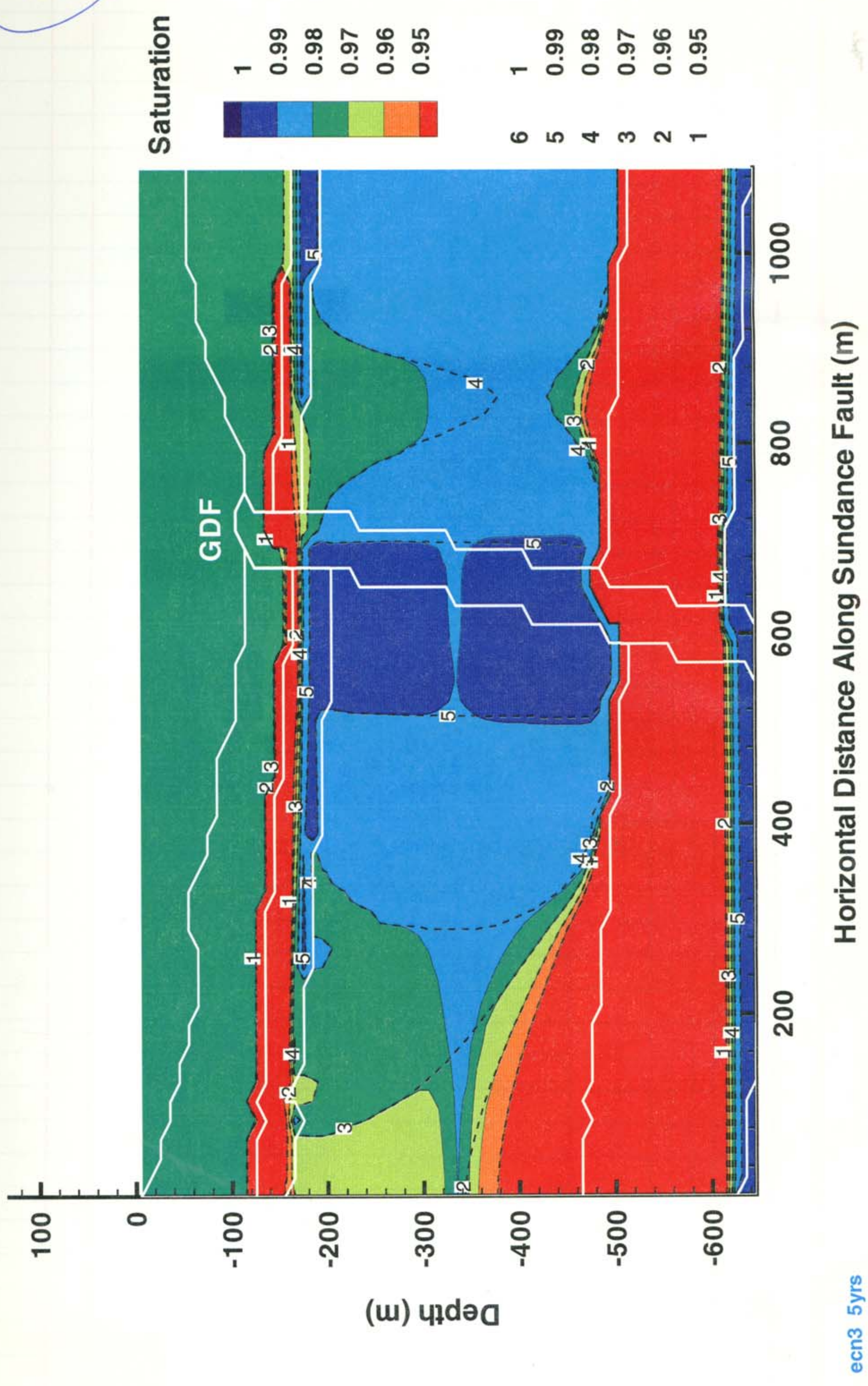
ECM3 steady state (isothermal case)
Infiltration rate: 30.59 mm/yr.
Dashed lines represent steady-state solution for ecm1 (.3 mm/yr case).



ecn3

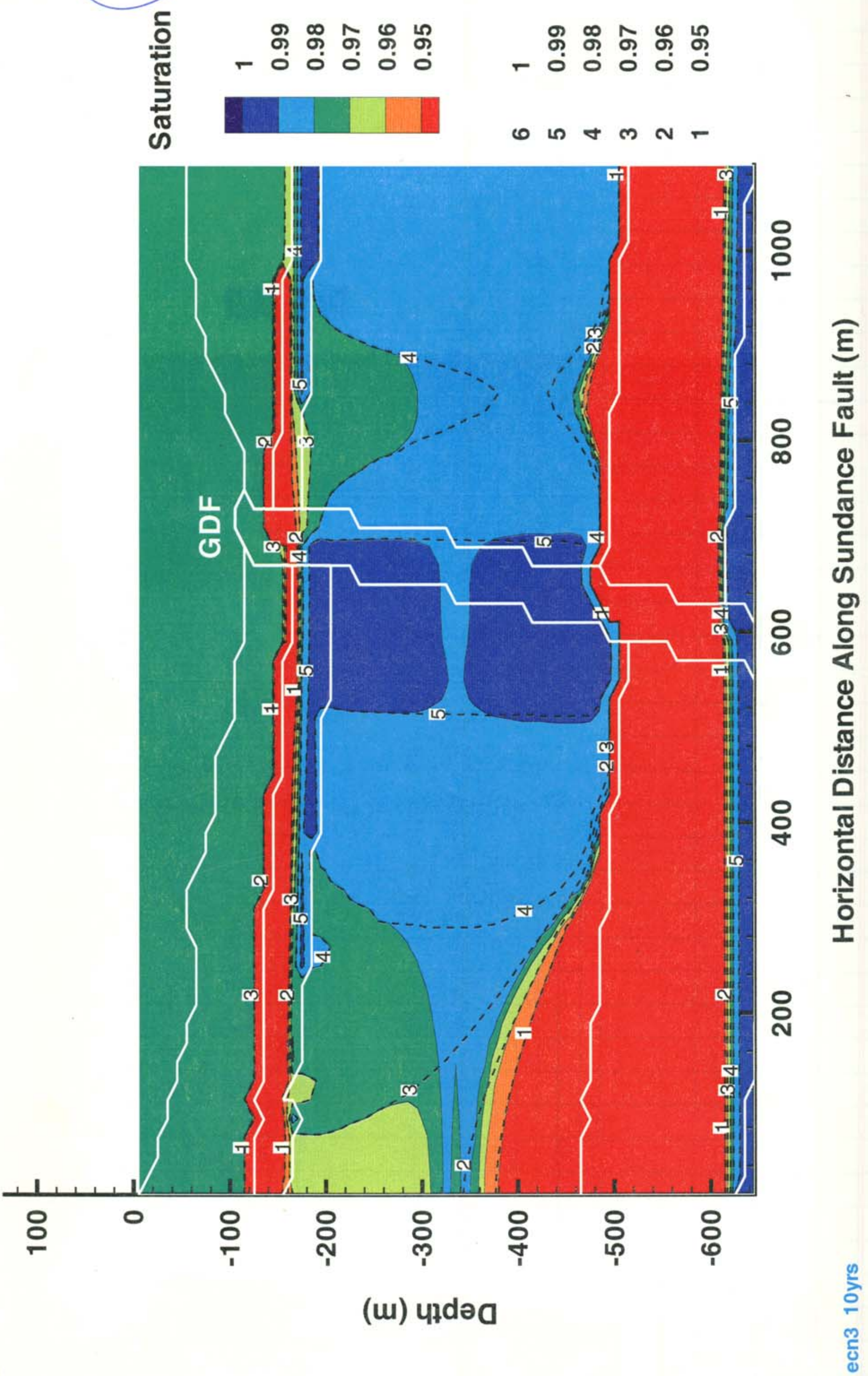
ECN3 after 1 yr of repository heating.
Infiltration rate 30.59 mm/yr
Dashed lines represent isothermal steady state solution.

GRD

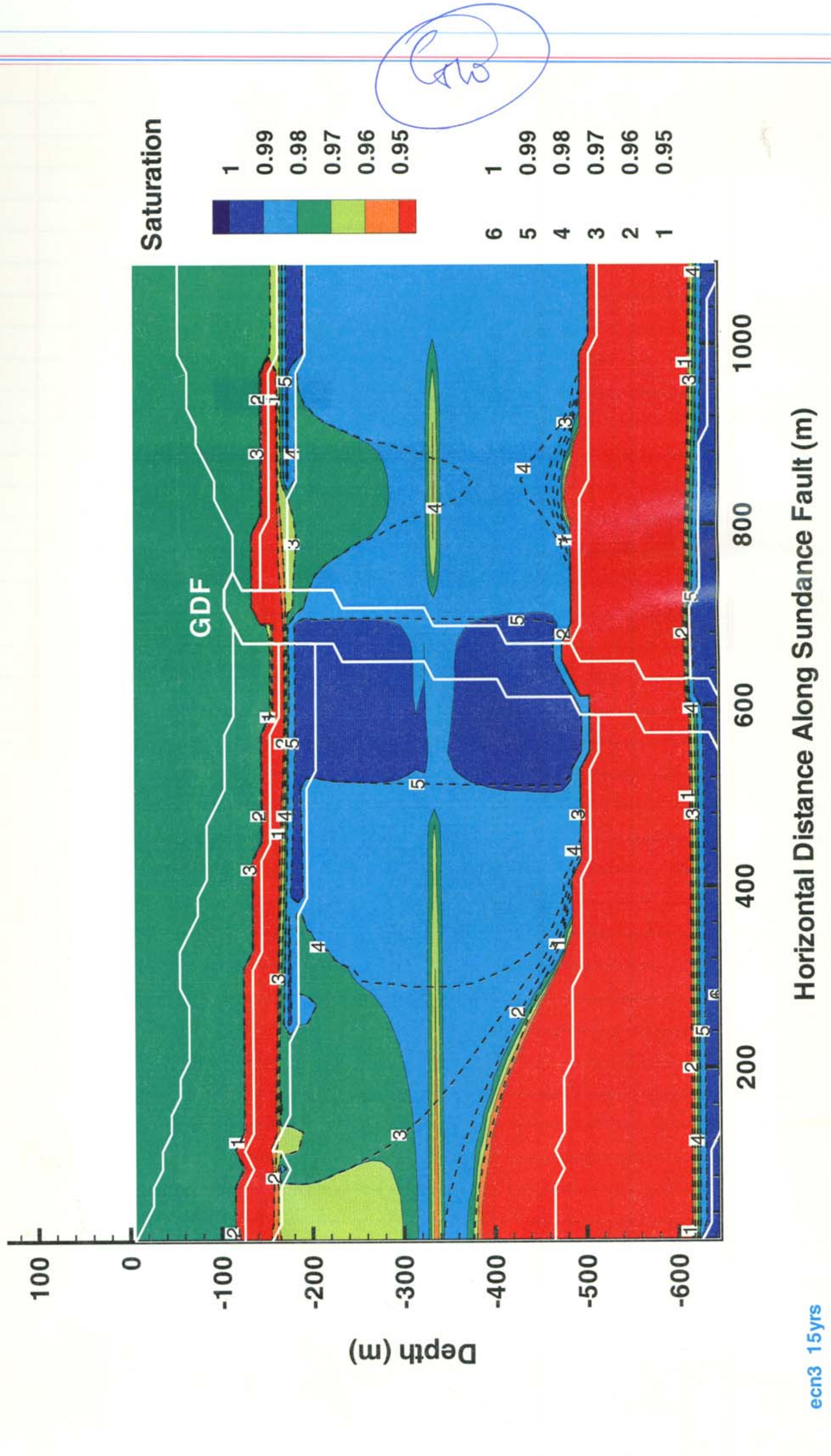


GRD

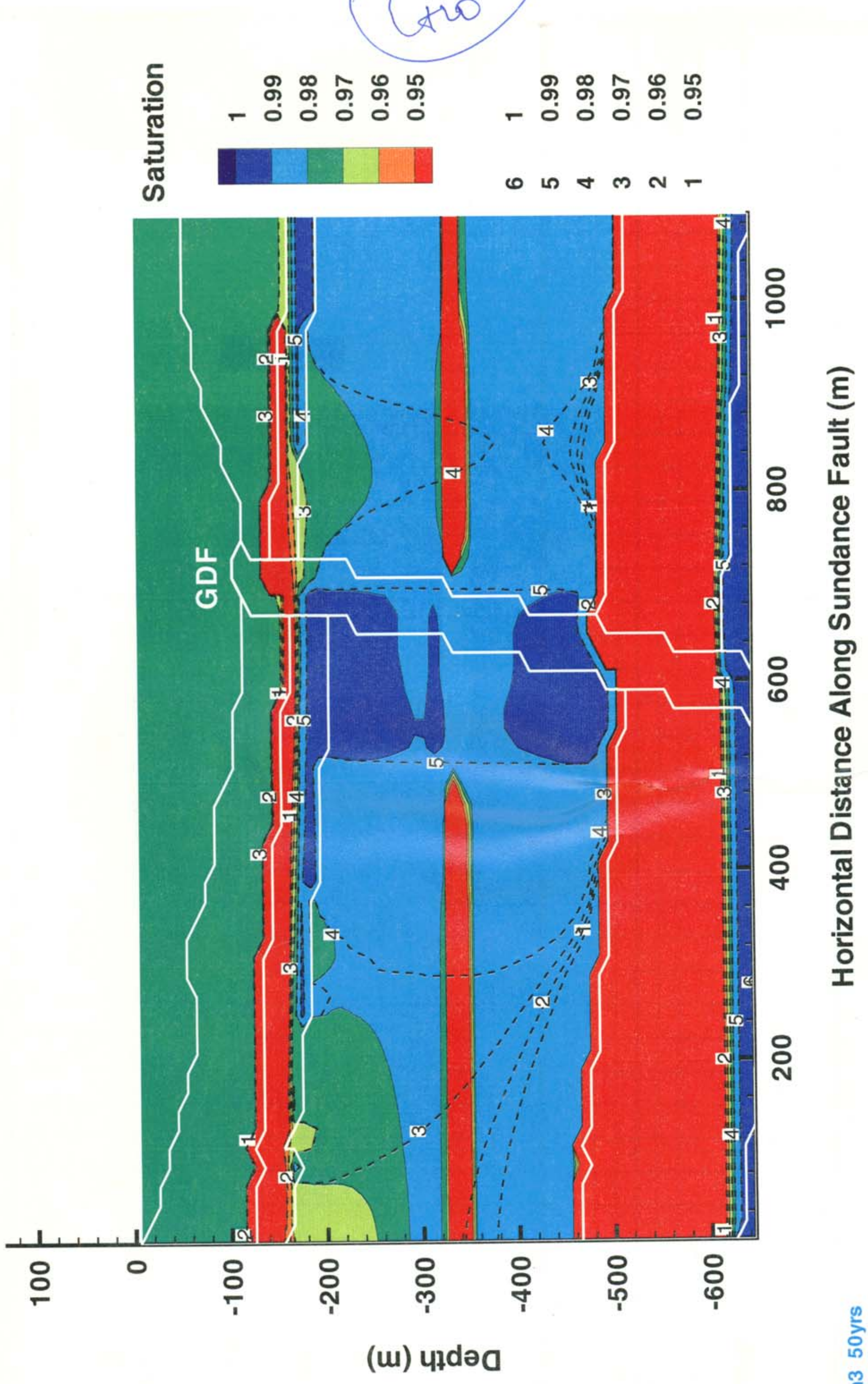
ECN3 after 5 yrs of repository heating
30.59 mm/yr infiltration
Dashed lines represent isothermal steady state solution.



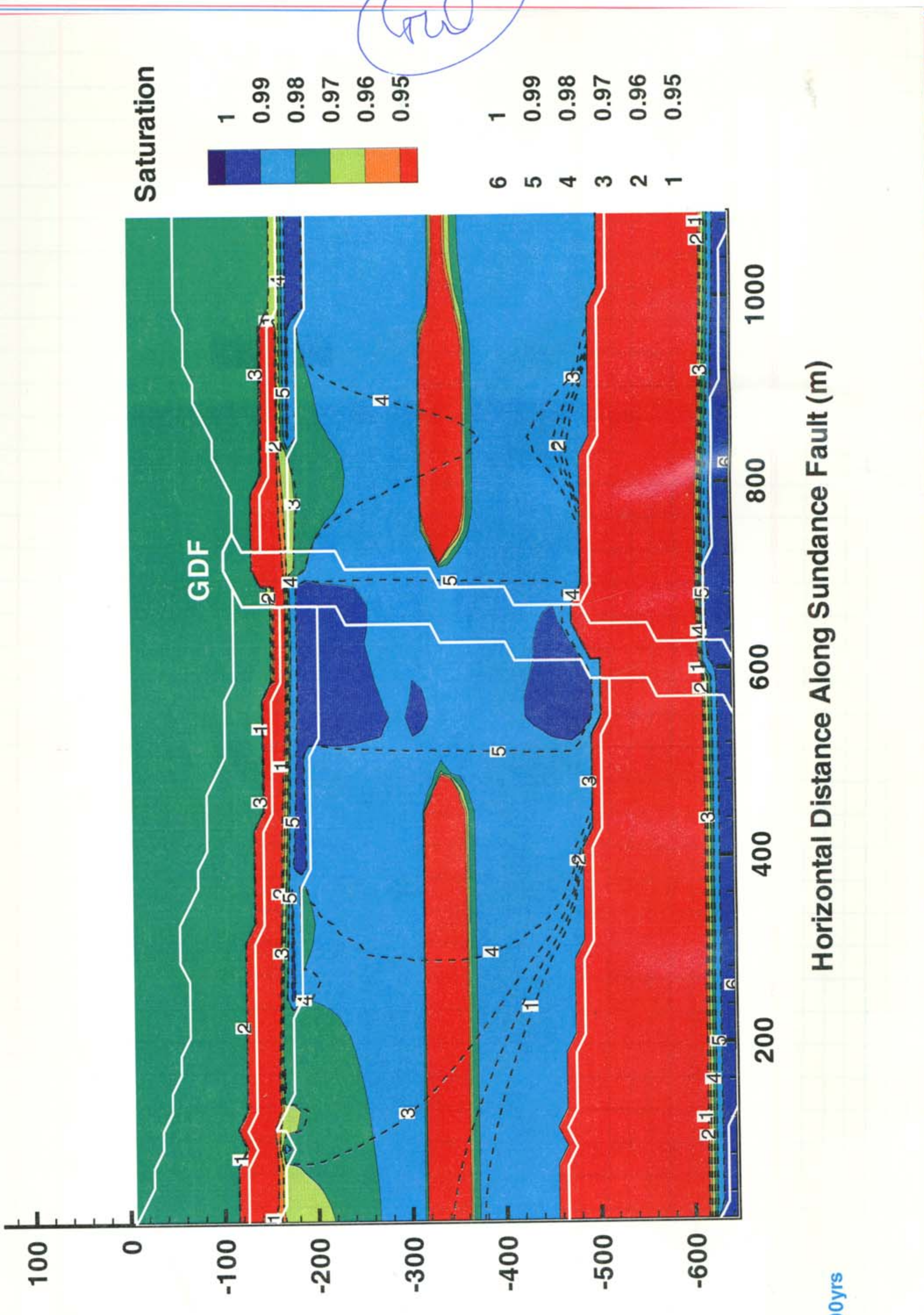
ECN3 after 10 yrs repository heating
30.59 mm/yr infiltration
Dashed lines represent steady state isothermal solution.



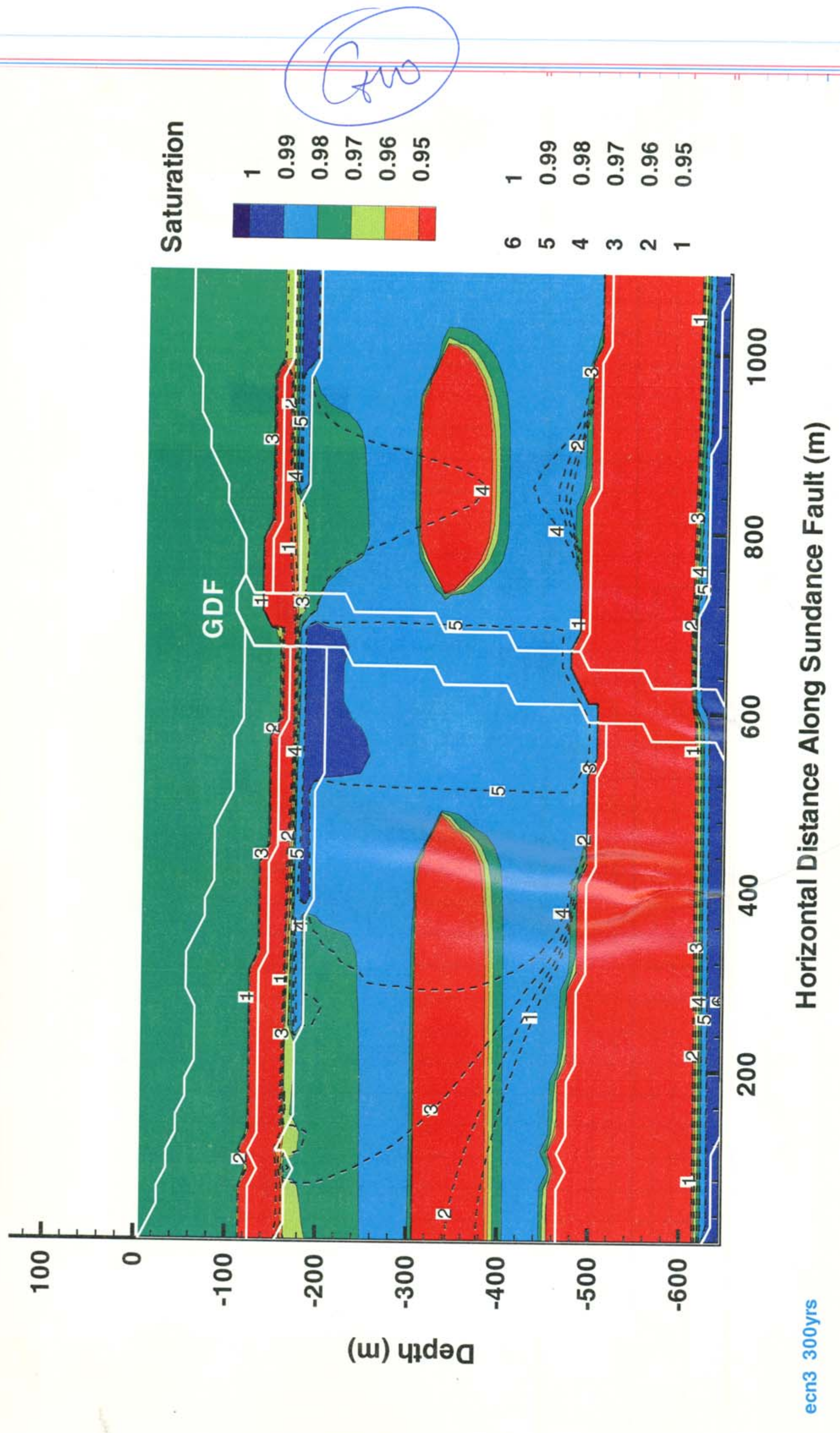
ECN3 after 15 yrs repository heating
30.59 mm/yr infiltration
Dashed lines represent steady state isothermal solution



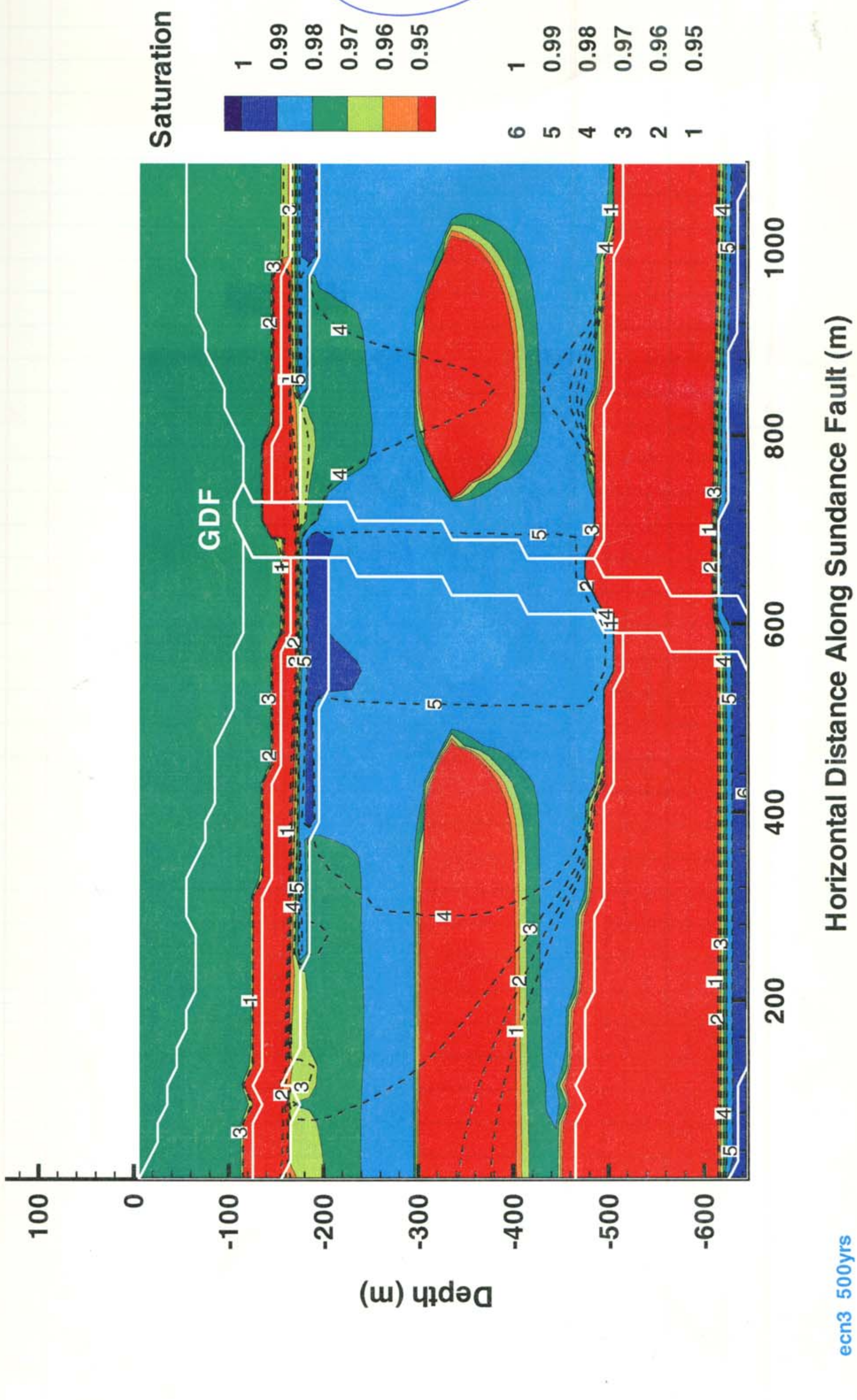
ECN3: 50 yrs of repository heating
30.59 mm/yr infiltration
Dashed lines represent steady state isothermal solution.



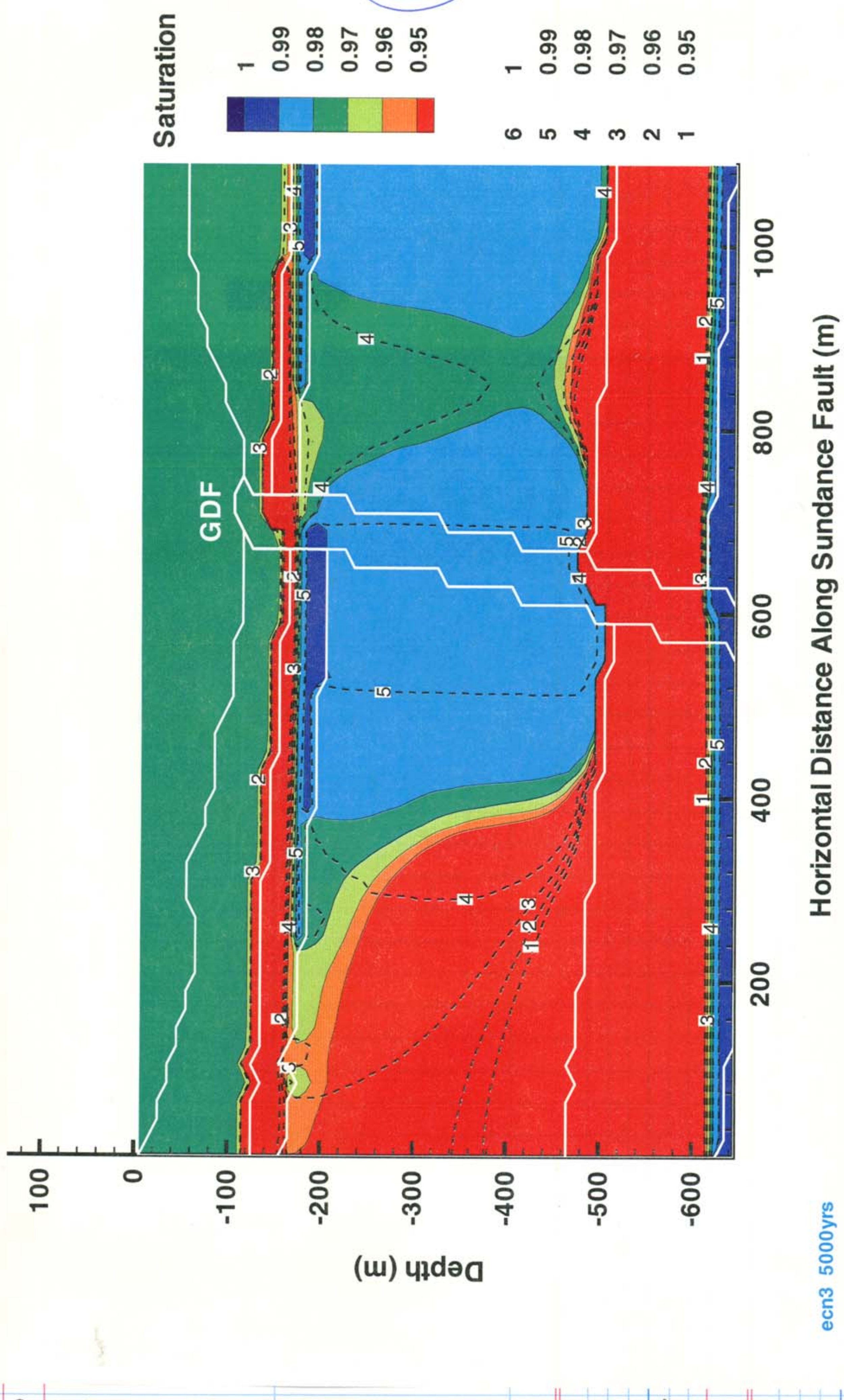
ECN3: 100 yrs of repository heating
30.59 mm/yr infiltration
Dashed lines represent steady state isothermal solution



ECN3 after 300 yrs of repository heating
30.59 mm/yr infiltration
Dashed lines represent steady state isothermal solution

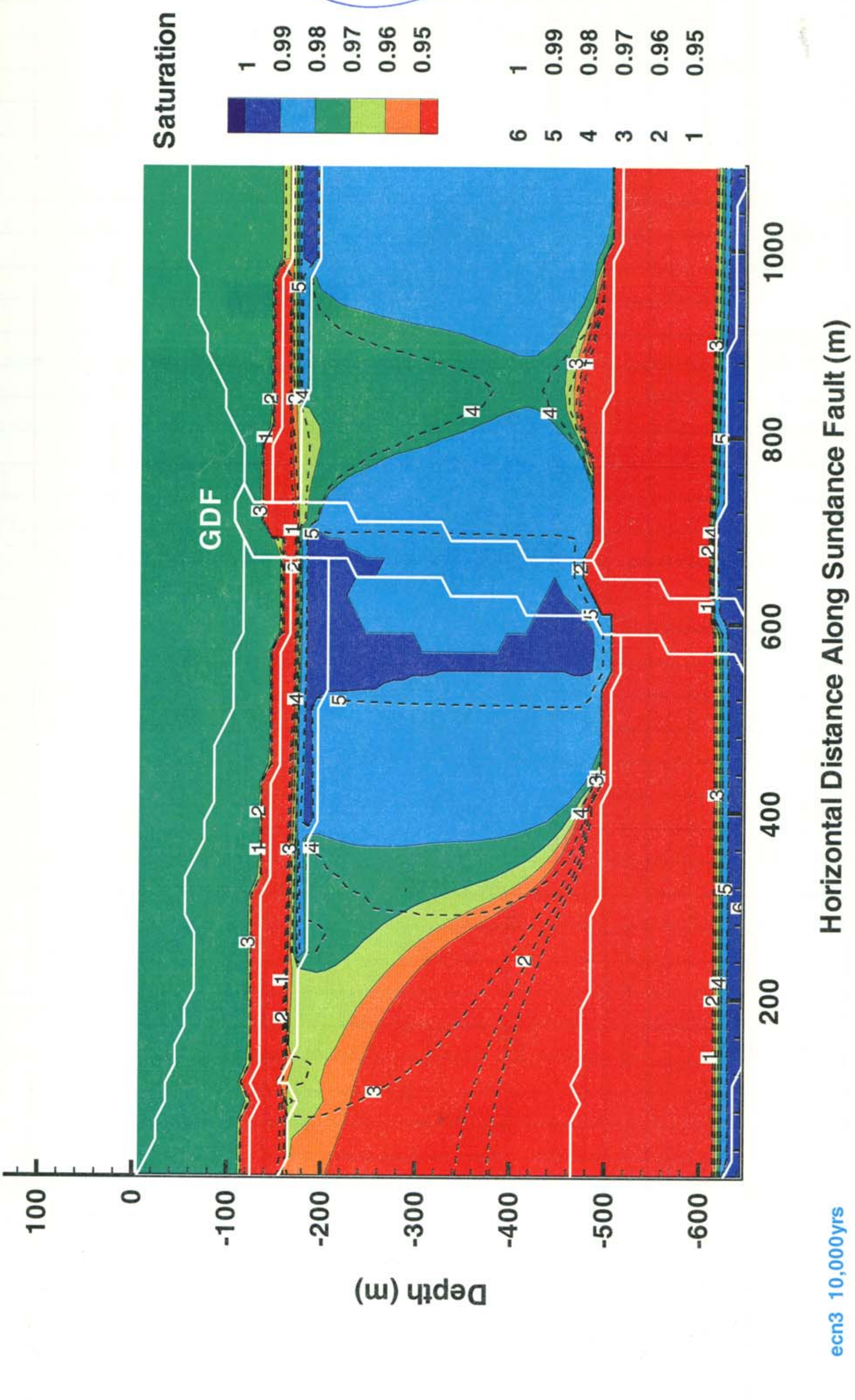


ECN3 after 500 yrs of repository heating
30.59 mm/yr infiltration
Dashed lines represent steady state isothermal solution



ECN3 after 5000 yrs of repository heating.
30.59 mm/yr infiltration
Dashed lines represent steady state isothermal solution.

GFW



ECN3 after 10000 yrs of repository heating
30.59 mm/yr infiltration
Dashed lines represent steady state isothermal solution.

Results of ECM3/ECN3 agree with those of ECM2/ECN3, which was summarized on p. 48.

(1) Isothermal steady-state solution (p. 49) shows the development of perched-water bodies in the PTn and TSw units. Both perched bodies have saturations ranging from 0.99 to 1.0 with positive pressure heads in the middle.

(2) Repository heating initially caused increase in the extent of the perched zone and increase in saturation within the perched zone. Dry-out of perched zone within the ~~TSw~~ TSw unit started at about 10 yrs and increased with time. Rewetting of the repository zone started ~~at about~~ while dry-out was still proceeding in surrounding areas.

(3) The PTn perched-water body remained essentially unchanged throughout the repository-heating period.

(4) Magnitudes of saturation are much larger in ECN3 results than in ECN2. Also, changes of saturation caused by heating are more noticeable for ECN3 than for ECN2.

All analyses up to now considered the fault (Ghost Dance Fault) only as a geometrical entity, which has an effect only because of the juxtaposition of different materials between the downthrown and upthrown blocks. The fault zone itself has hitherto been assigned the same properties as the adjasent rock blocks. Additional analyses were conducted to examine the effects of assigning different properties to the fault zone.

Properties of fault-zone material were assigned within the equivalent-continuum concept. First the fault zone was considered to have higher fracture density than surrounding blocks. Next it was considered that the higher fracture density can be translated into higher fracture porosity, which implies

higher bulk permeability using the equivalent-continuum concept.

The additional cases ~~analyzed~~ were distinguished through the ratio k where

$$k = \frac{\text{fault-zone fracture density}}{\text{rock-block fracture density}}$$

which gives a fault-zone fracture porosity of $k\phi_f$ where ϕ_f is the fracture porosity of surrounding blocks. The different cases and their k values and infiltration rates are described in the table below. Cases ECM1/ECN1, ECM2/ECN2, and ECM3/ECN3 all have $k = 1$, as the table shows.

GRO

GRO

ECM Analysis Cases

Case ID	Infiltration rate (mm/yr)	(k) Fault-zone fracture density ratio	Input file name (.dat extension) Isothermal to steady state	Nonisothermal with heat source
1	0.3	1.0	ecm1	ecn1
2	3.0	1.0	ecm2	ecn2
3	30.0	1.0	ecm3	ecn3
f1	0.3	10.0	ecmf1	
f2	3.0	10.0	ecmf2	ecnf2
f3	30.0	10.0	ecmf3	
f4	0.3	100.0	ecmf4	
f5	3.0	100.0	ecmf5	*
f6	30.0	100.0	ecmf6	
f7	0.3	500.0	ecmf7	
f8	3.0	500.0	ecmf8	*
f9	30.0	500.0	ecmf9	

GRO

GRO

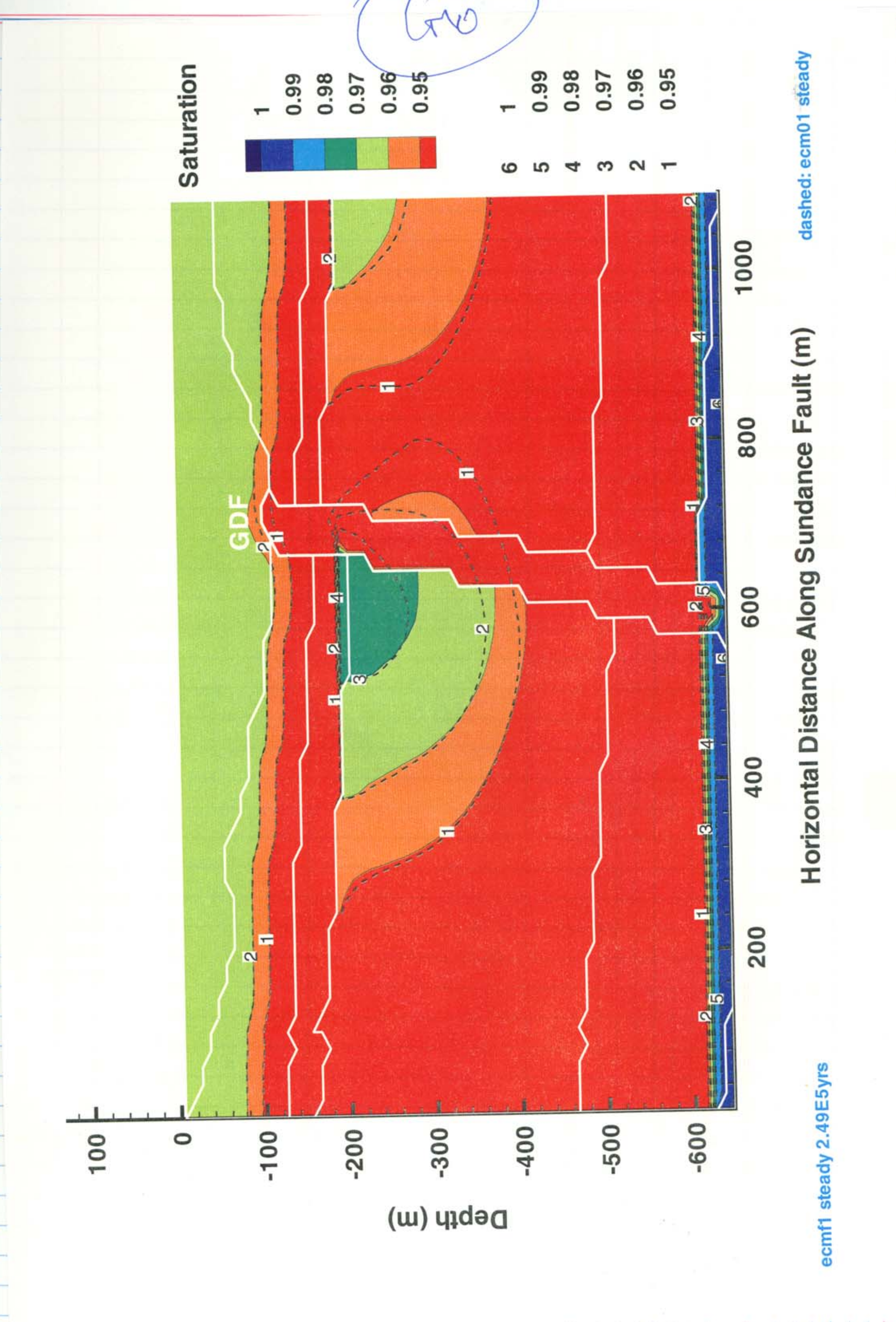
ecmf1, ecmf2, ecmf3

0.3, 3.0, 30.0 mm/yr infiltration respectively (approximately).

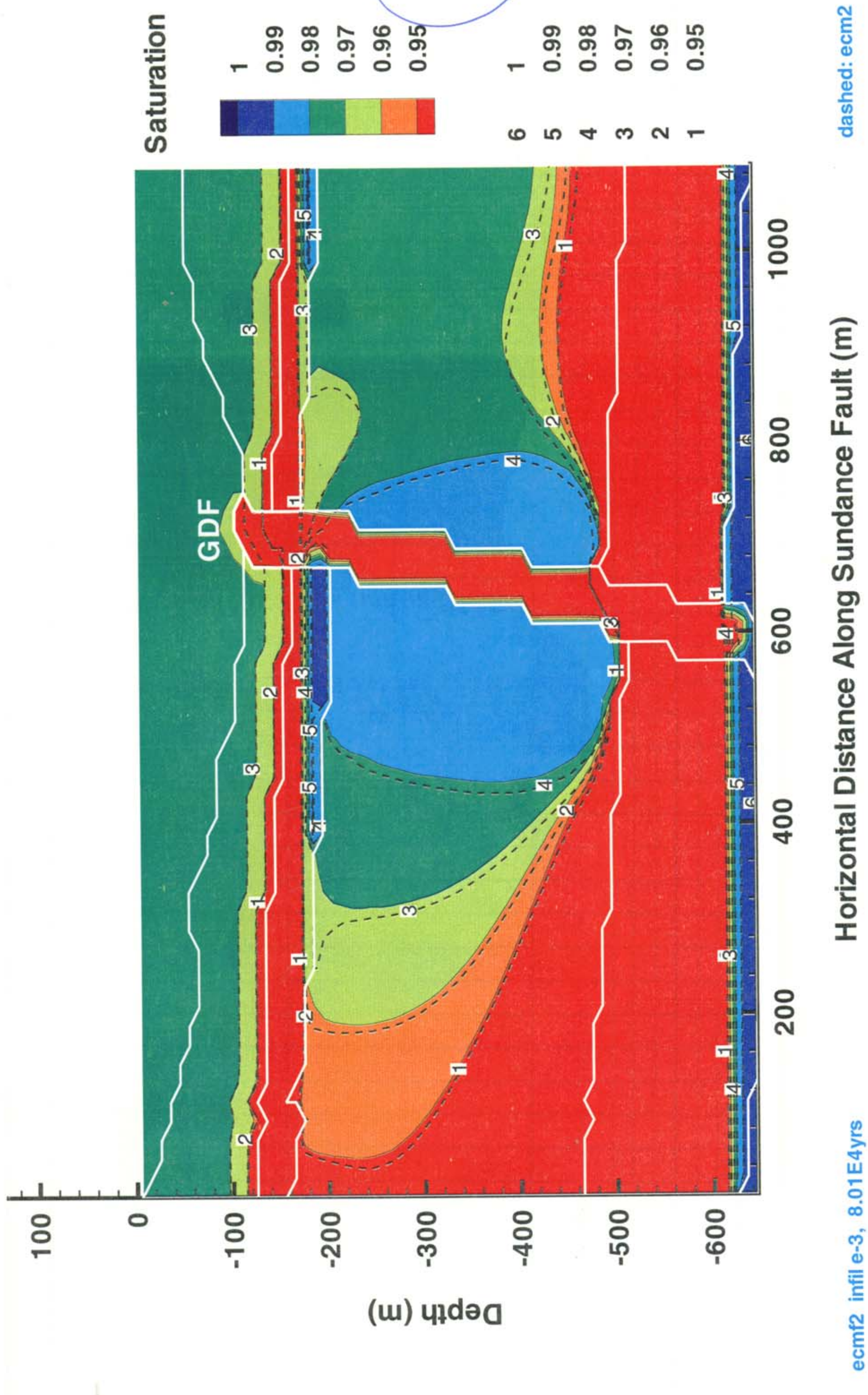
k = 10.0 in each case. That is, fracture porosity within GDF zone is 0.018 in each case, which is 10 times the fracture porosity of 0.0018 ~~for the~~ surrounding rock blocks.

Results for ecmf1, ecmf2 and ecmf3 compare with results for ecm1 (p. 30), ~~ecm~~ ecm2 (p. 38) and ecm3 (p. 49), respectively ~~;~~ i.e., the corresponding k=1 cases as described on p. 61. The results of ecmf1, ecmf2 and ecmf3 are presented on p. 63, 64, and 65. They all show that the effect k=10 (compared to k=1 cases) ~~is~~ G10 ~~essentially lower~~ consists of lower saturation within the fault zone. That is, the increased fault-zone fracture density causes decreased water saturation (increased drainage) of the fault zone.

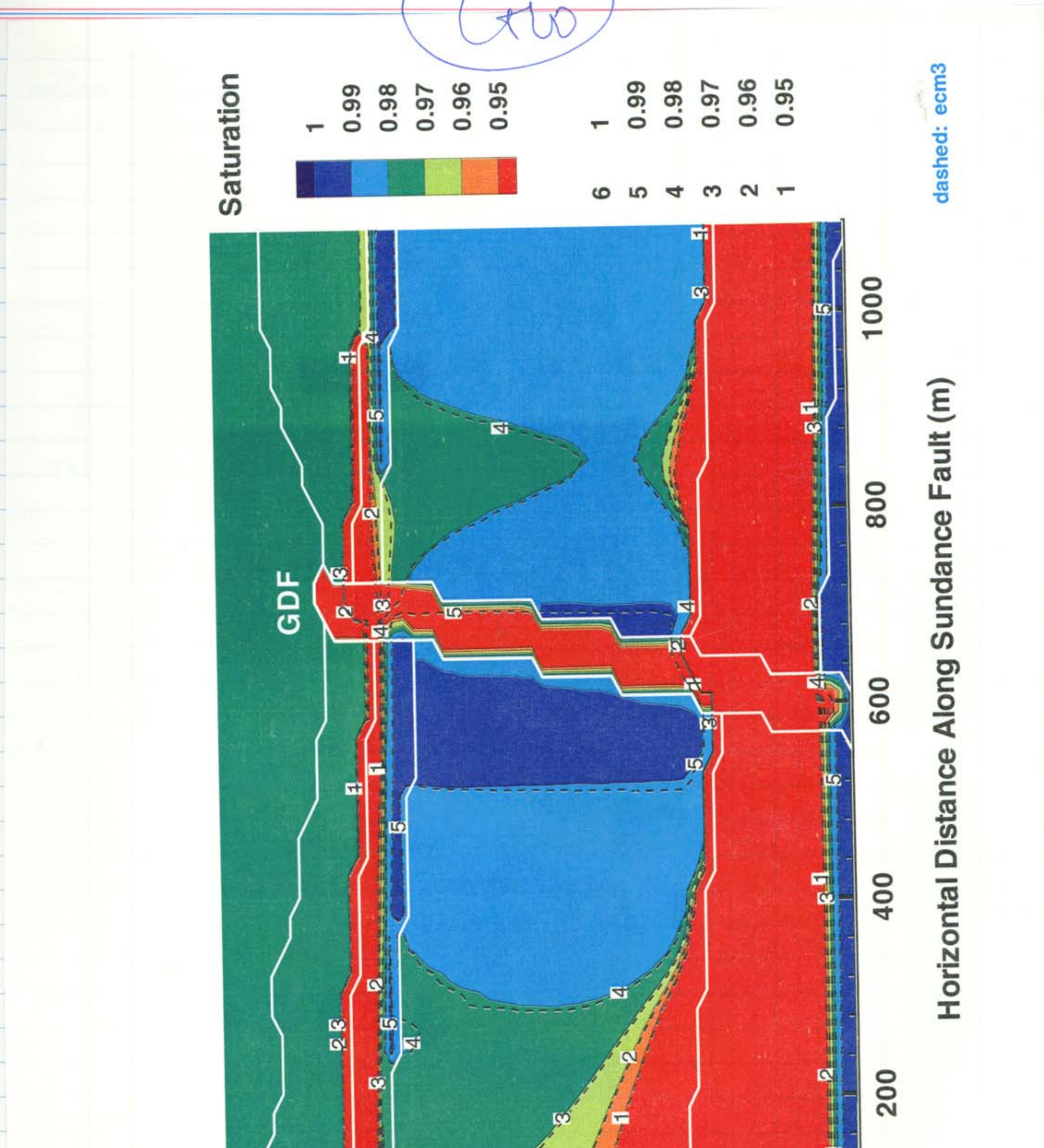
Lower saturations also occur in the adjasent blocks, ~~but drainage of the adjas~~ G10 but not to the extent that might be expected. Drainage of faulted blocks by the increased fracture density of the fault zone is impeded by capillary barrier along the walls of the fault zone. Such ~~ba~~ capillary barrier is broken at the higher saturation that occurs G10 ~~under 30~~ in the perched-water bodies under 30 mm/yr infiltration. Therefore, drainage of faulted blocks due to increased fault-zone fracture density occurs most in the 30 mm/yr case and least in the 0.3 mm/yr case.



ecmf1 : k = 10 , infiltration ≈ 0.3 mm/yr.
Isothermal steady-state solution.
Equivalent k = 1 case on p. 30, which is shown as dashed lines on this plot.



ecmf2: k=10 infiltration ≈ 3 mm/yr
Isothermal steady state solution. Dashed lines represent case with k=1 (see also p. 38).



ecmf3: k=10, infiltration rate ≈ 30 mm/yr.
Steady state isothermal solution. Dashed lines
represent equivalent k=1 case (see also p. 49).

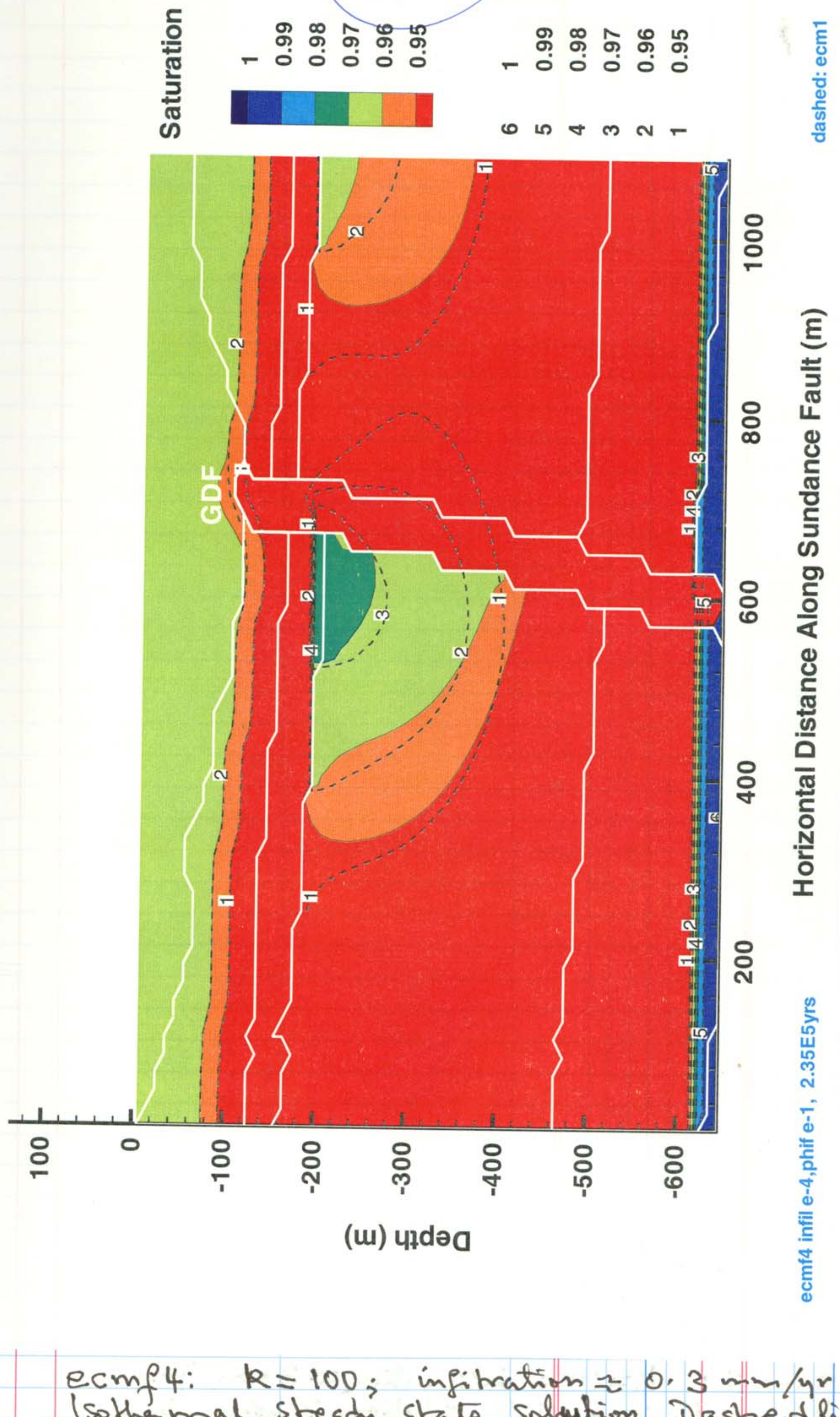
Additional results of the k>1 cases are presented in the next six pages. Examination of the k>1 steady-state isothermal cases lead to the following observations:

(1) Increased fault-zone fracture density causes reduced saturations within the fault zone

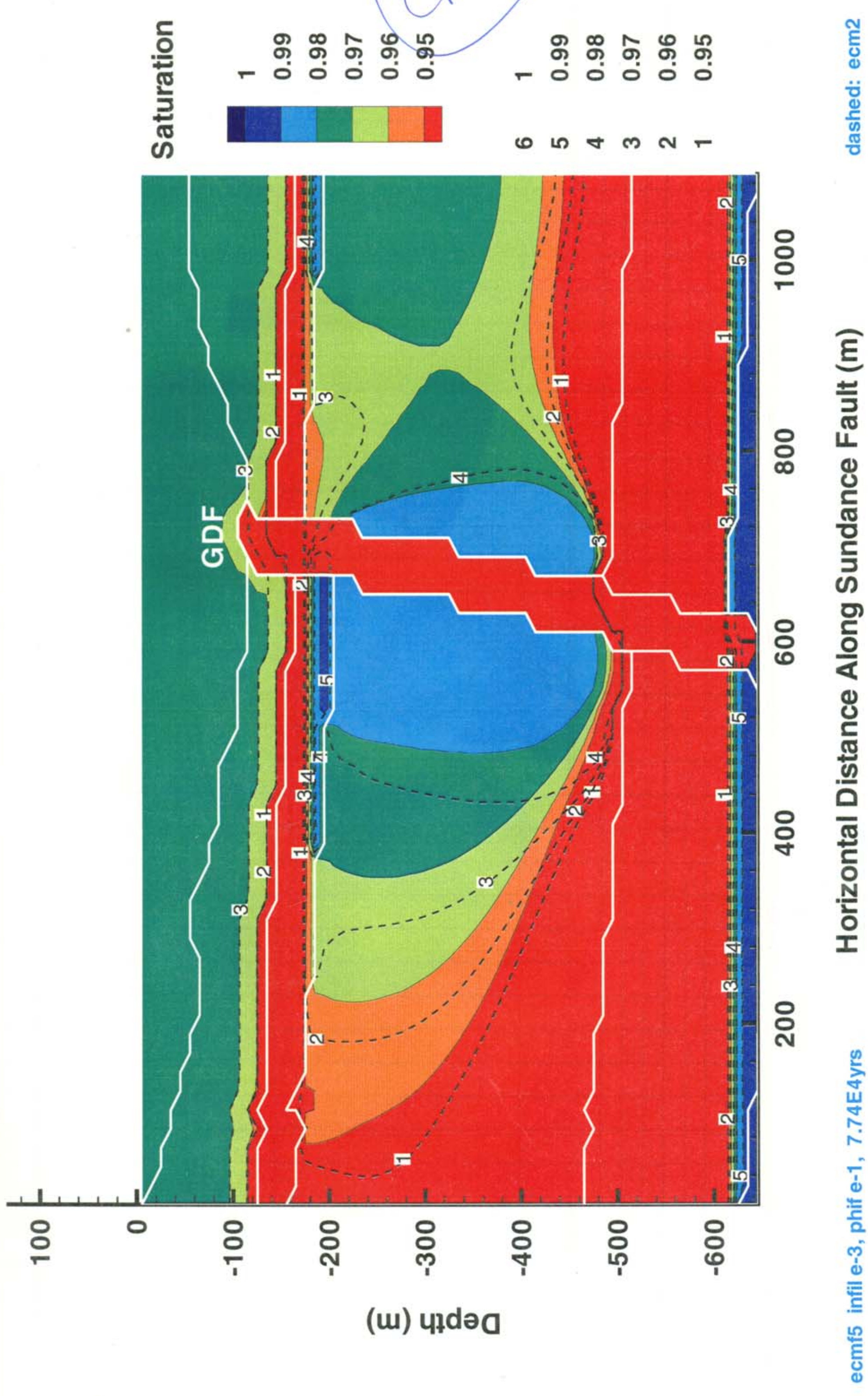
(2) Drainage of faulted blocks (leading to saturations smaller than in corresponding k=1 case) occurs in all k>1 cases. The extent of faulted-block drainage increases as k increases.

(3) Faulted-block drainage is impeded by capillary barrier in fault zone to fault block transition area. As a result, the extent of fault-block drainage increases as infiltration rate increases, because of reduction of capillary-barrier strength at higher infiltrations.

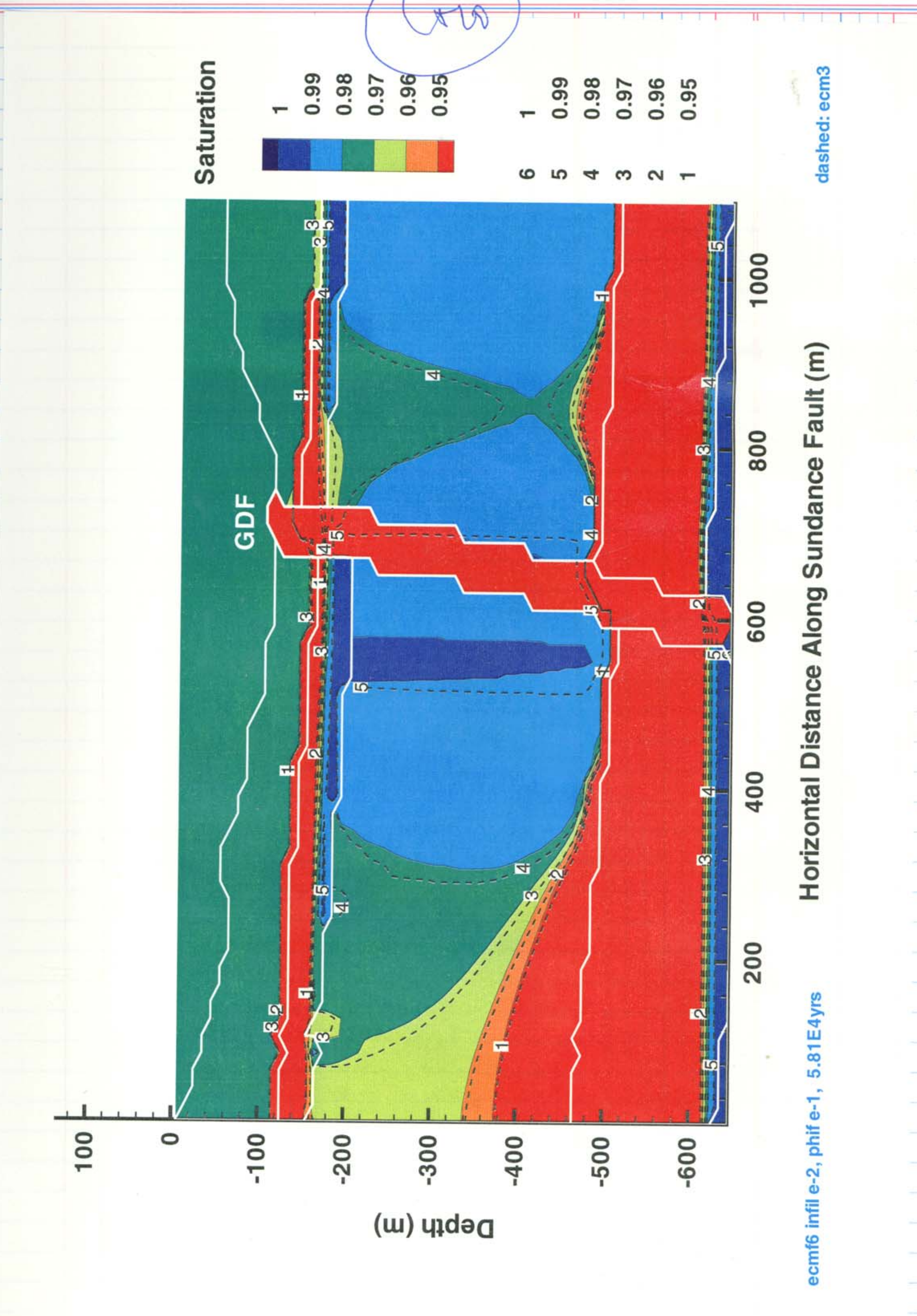
(4) The perched-water body that occurs at the base of the down-thrown PTn block ~~is not drained by~~ (G10) remains essentially unchanged as k is increased from 1 to 500, except that the portion of the perched body that occurs inside the fault zone in k=1 cases is drained in all k≥10 cases.



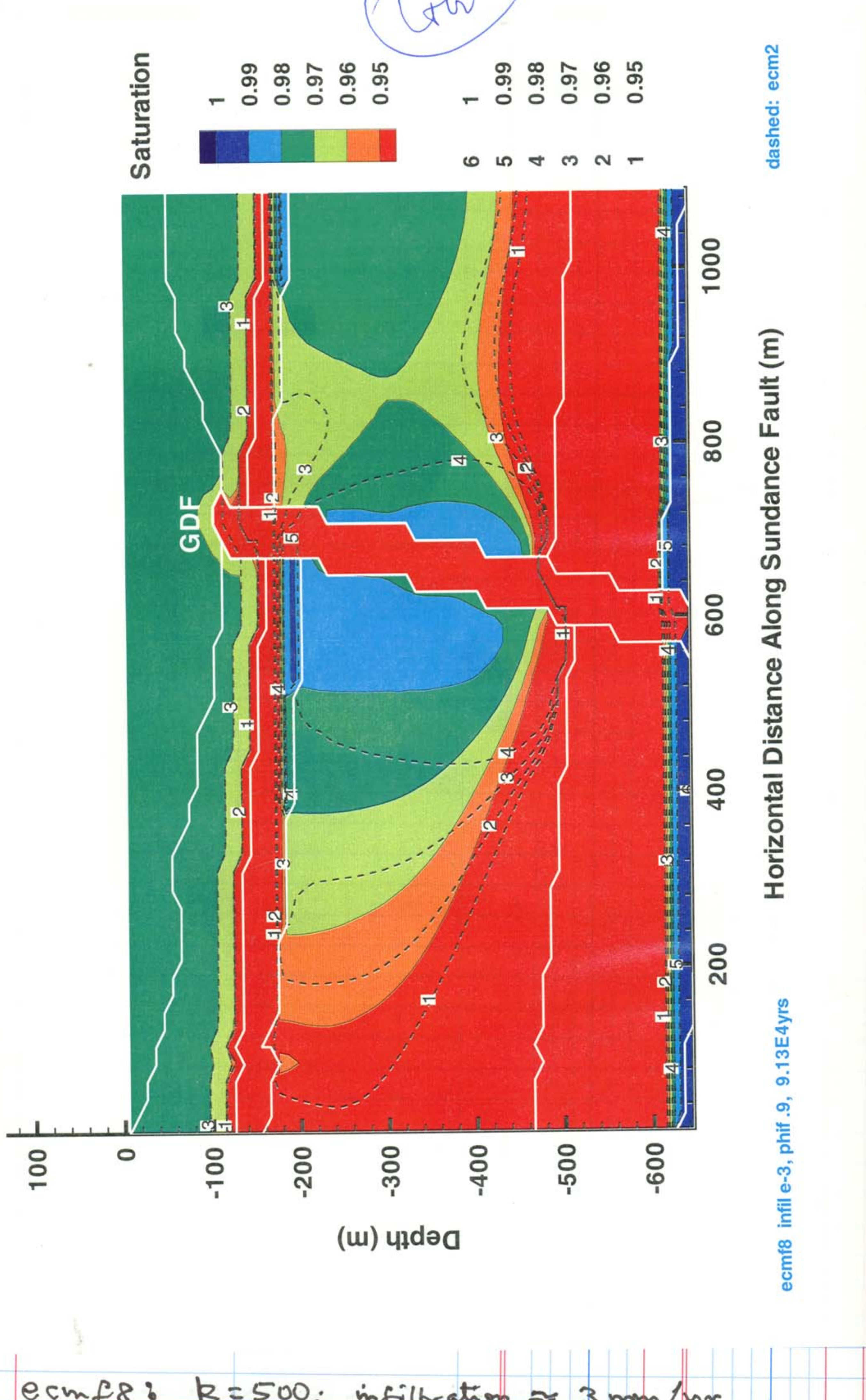
ecmf4: k = 100; infiltration ≈ 0.3 mm/yr
Isothermal steady state solution. Dashed lines
represent equivalent k=1 case.



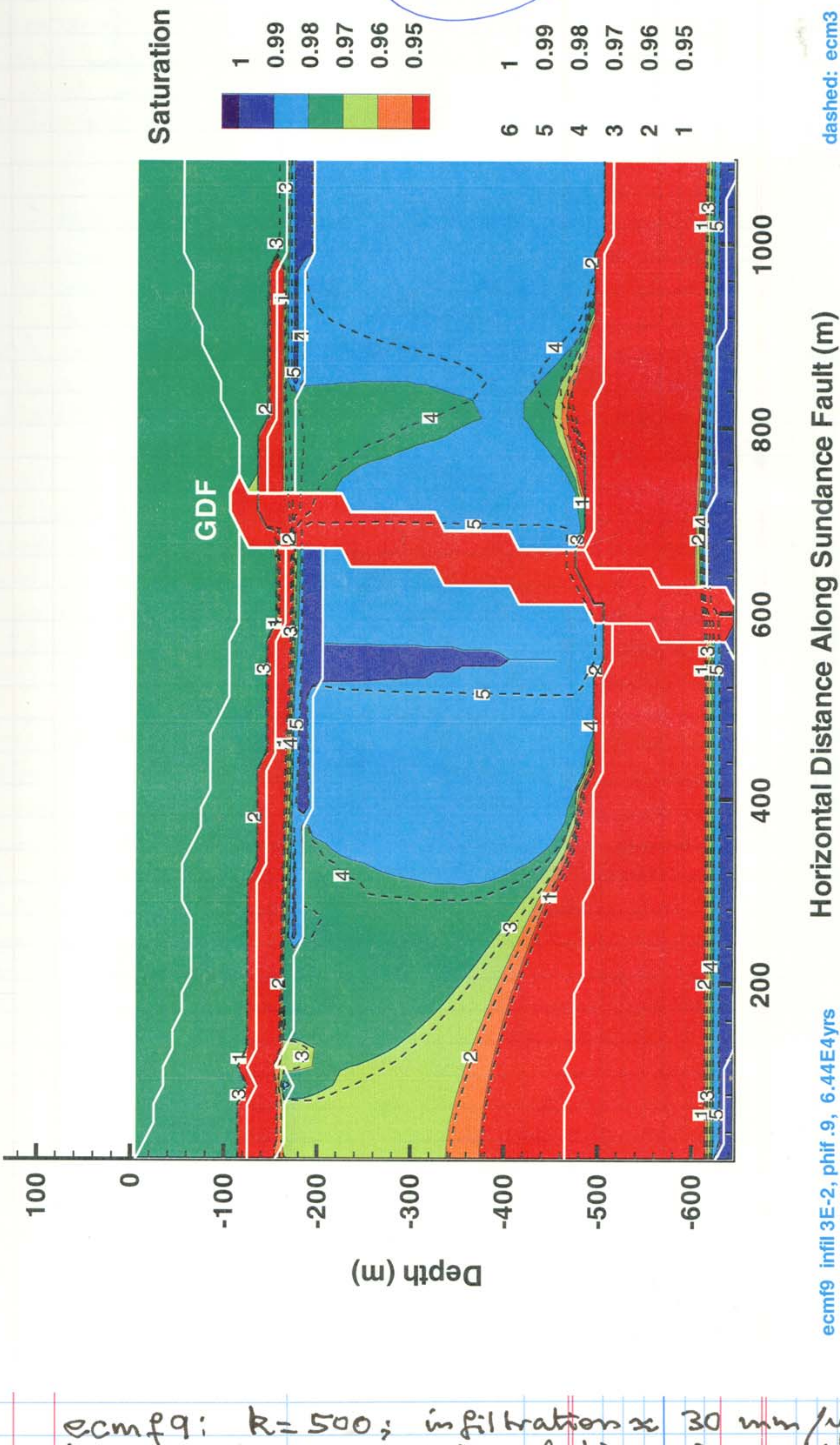
ecmf5 : k=100; infiltration ≈ 3 mm/yr.
Isothermal steady state solution. Dashed lines represent k=1 case.



ecmf6 : k=100 ; infiltration ≈ 30 mm/yr
Isothermal steady-state solution. Dashed lines
represent k=1 case.



ecmf8: k=500; infiltration ≈ 3 mm/yr
Isothermal steady-state solution. Dashed lines
represent k=1 case



ecmf9: k=500; infiltration ≈ 30 mm/yr
Isothermal steady-state solution. Dashed lines represent case of k=1.

ECNF2

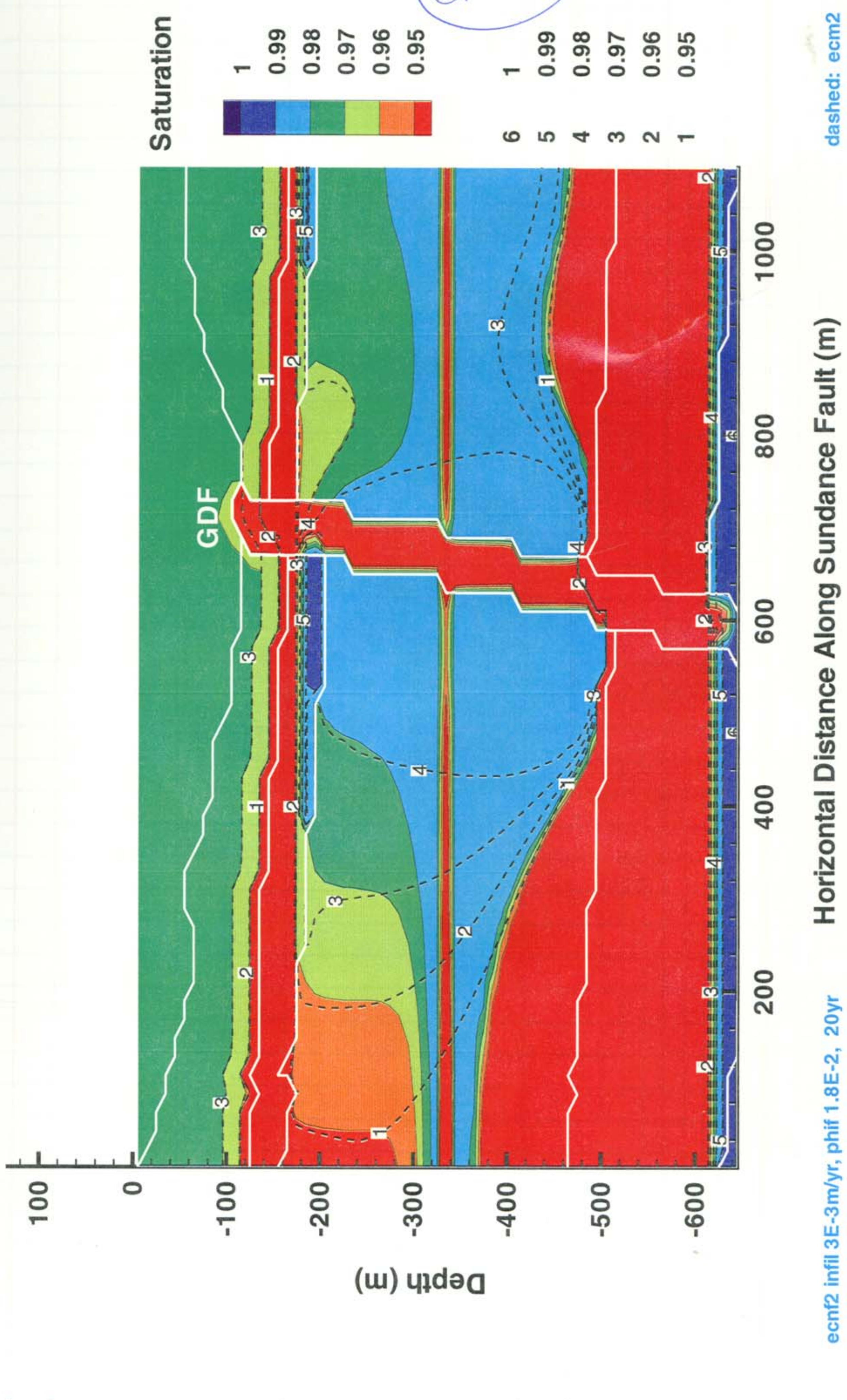
Non-isothermal analysis with k=10 and 3 mm/yr infiltration. Results of ecnf2 (p. 64) for the initial conditions for this case. The results are presented in the next five pages. The following observations are made:

(1) Comparison of ecnf2 results with ~~enc~~ ecn2 results (presented on p. 39-47) shows that drainage of the fault-zone is the only noticeable difference caused by the change from k=1 to k=10 for the 3 mm/yr infiltration case. Corresponding ecn2 and ecnf2 saturation contours are essentially the same.

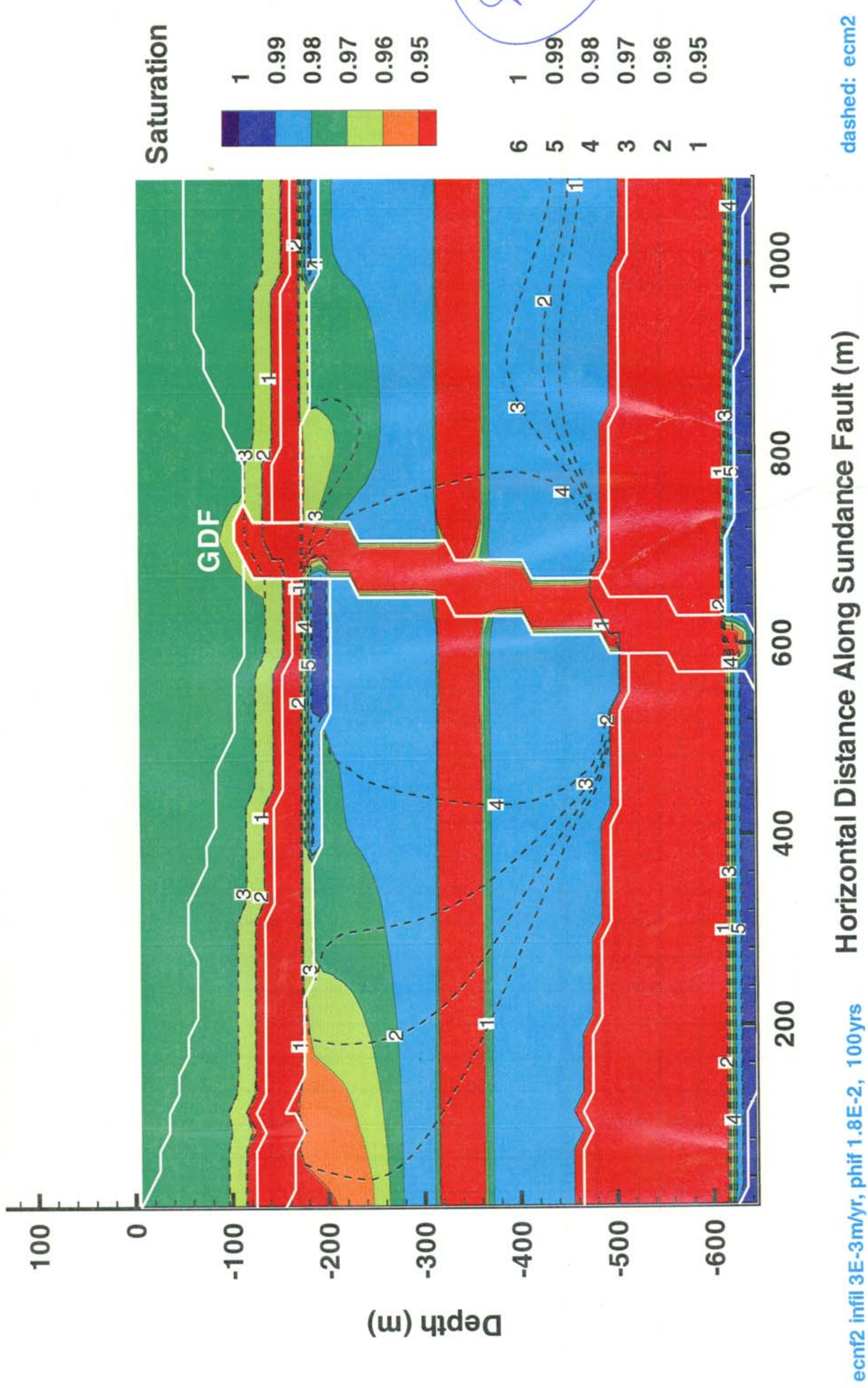
(2) Introduction of repository heating causes increase in size of TSw petched-water zone. The increased continued, upward, downward, and laterally until about 100 yrs. Decrease in size of petched zone started at about 500 yrs.

(3) At the same time, dry-out, i.e., ~~decrease~~ decrease in saturation, started at the repository horizon after about 20 yrs. The dry-out zone grew upward and downward~~, reaching maximum distance from repository~~. It continued to grow, even after rewetting has begun in some area: re-wetting of ~~zones~~ TSw zones under the PTn perched body was proceeding at the same time that dry-out was growing at other locations.

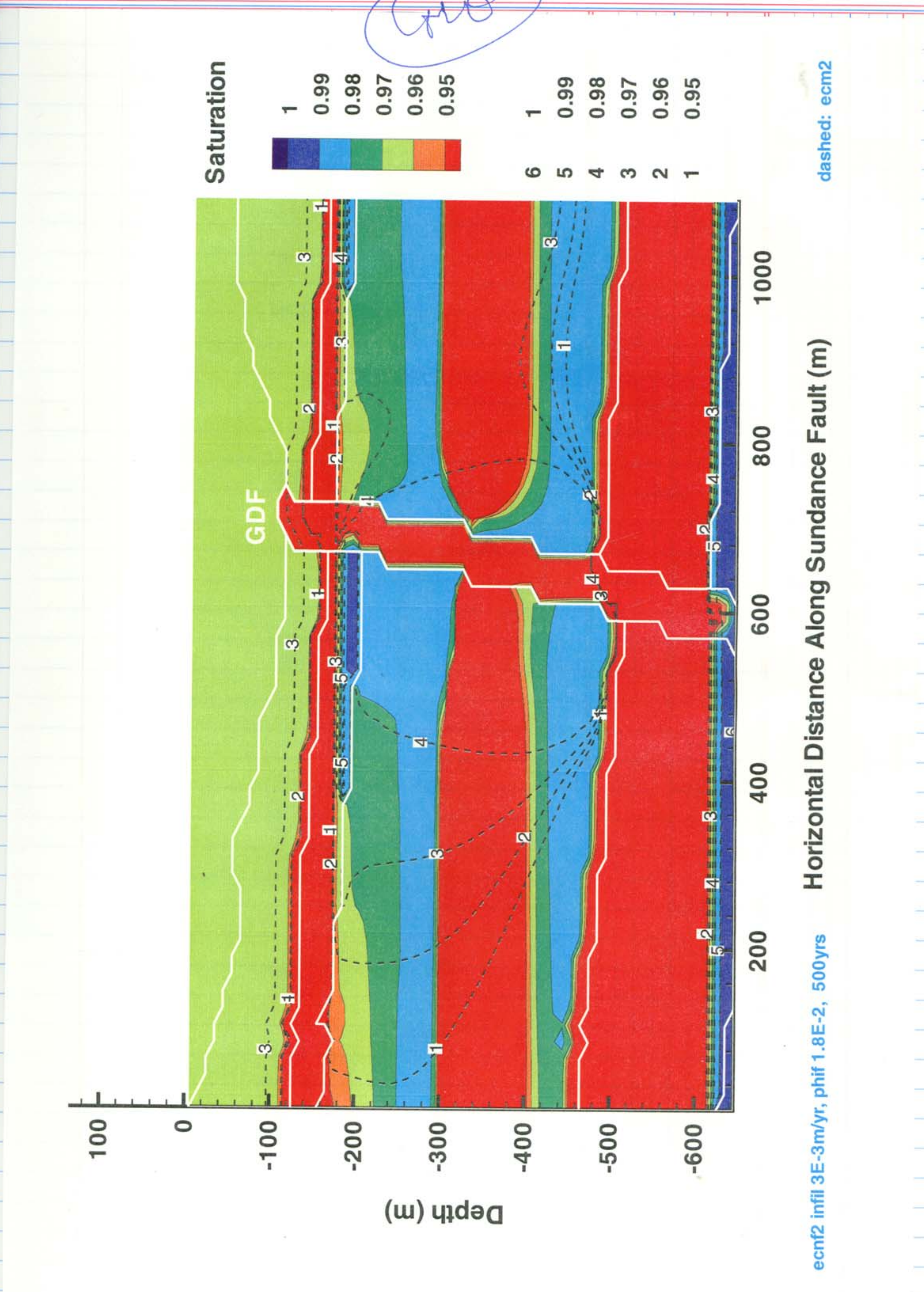
(4) PTn perched-water body is essentially unaffected by repository heating.



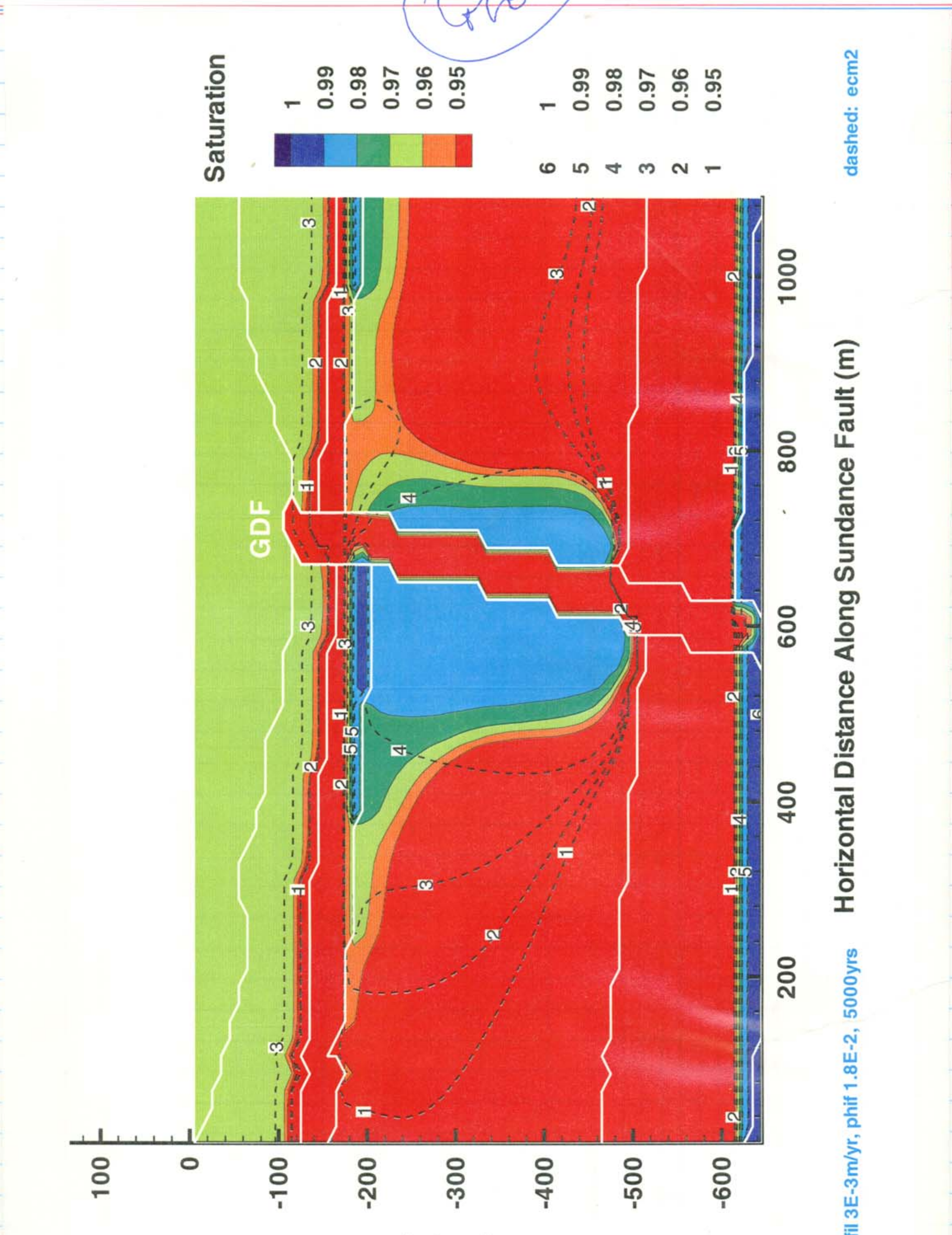
ecnf2 after 20 yr of repository heating.
k=10 infiltration ≈ 3 mm/yr.



ecnf2 after 100 yrs of repository heating
k=10 infiltration ≈ 3 mm/yr



ecnf2 after 500 yrs.



ecnf2 after 5000 yrs.

~~Entries Continued at Notebook #188 Vol. 3~~

AHC 7/15/99

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding procedures used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

[signature]
7/05/99