MUFITS

Multiphase Filtration Transport Simulator
version 2013.B

Example-H2

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Contents

1 Example-H2

1.1. Introduction

This example is based on the 10th SPE comparative solution project reservoir [1]. The simulation results are published in [2] (2D problem).

By reviewing this example-H2, you are expected to learn the basic principles of how to:

- specify a 3D Cartesian grid and the extension of the grid cells;
- make a region of the reservoir inactive;
- load heterogeneous petrophysic data from an include file;
- specify local grid refinement;
- impose Dirichlet boundary conditions;
- operate on arrays (specify linear distribution of pressure).

1.2. The problem formulation

We consider the 50th layer of the 10th SPE reservoir (Fig. 1.1).

The layer is initially saturated with pure water. The initial distribution of the temperature is uniform. Hot CO_2 injected through the left boundary (y=0m). The parameters at the left (y=0m) and at the right boundary (y=1676.4 m) are fixed (Dirichlet boundary conditions). The boundaries x=0 m and x=457.2 m are impermeable. The initial pressure distribution is a linear function between the values at the boundaries (y = 0 m and y =

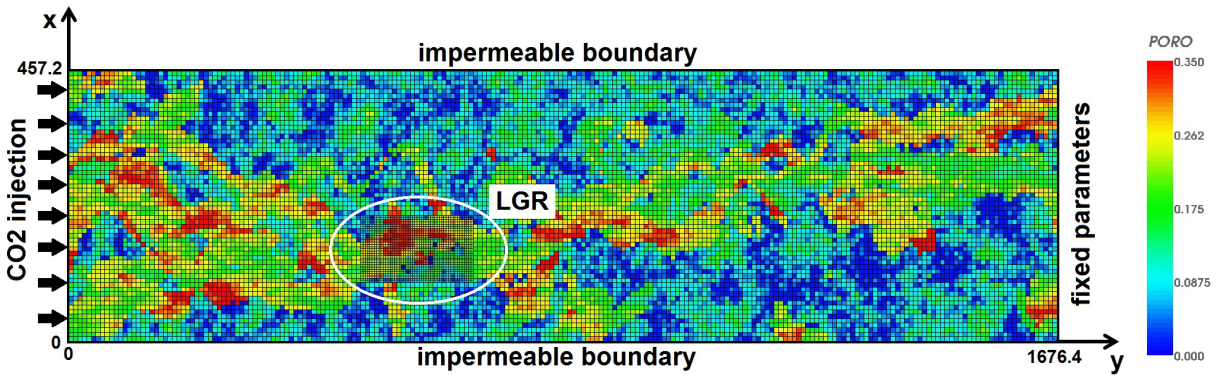

Figure 1.1: The schematic view of the problem. The porosity distribution is on the background.

1676.4 m). Thus CO_2-H_2O mixture flows from the left to the right through highly permeable zones - channels in the porous media. The channels in the layer are clearly visible through the porosity distribution (Fig.1.1). The heat conduction is neglected. The problem task is to calculate the parameters of the flow in the layer for 50 years period of injection. The parameters of the problem are summarized in the following table.

The parameters of the problem		
Domain	-	Rectangular area $X \in [0, 457.2]\ m$, $Y \in [0, 1676.4]\ m$;
Porosity	-	50th layer of the 10th SPE;
Permeability	-	Heterogeneous. 50th layer of the 10th SPE;
Grain density	-	$2500\ kg/m^3$;
Rock heat capacity	-	$1\ kJ/(kg \cdot K)$;
Relative permeabilities	-	Brooks and Corey (1964); $f_{H_2O} = \tilde{s}^4_{H_2O}$; $f_{CO_2} = (1 - \tilde{s}_{H_2O})^2(1 - \tilde{s}^2_{H_2O})$;
H_2O-rich phase critical saturation	-	0.2;
CO_2-rich phase critical saturation	-	0.05;
Initial pressure distribution	-	Linear function between the values at the boundaries ($y = 0\ m$ and $y = 1676.4\ m$);
Initial reservoir temperature	-	$295.15\ K$ $(22\ C)$;
Initial CO_2 molar fraction	-	0.0 (reservoir is saturated by pure water);

Pressure at the boundary $y = 0m$ (constant)	-	7.5 MPa;
Pressure at the boundary $y = 1676.4\,m$ (constant)	-	4.5 MPa;
Temperature at the boundary $y = 0\,m$ (constant)	-	320.15 K (47 C);
CO_2 molar fraction at the boundary $y = 0\,m$ (constant)	-	1.0 (pure CO_2 is injected).

1.3. Grid

According to the description of the 10th SPE reservoir [1] we use uniform grid with 60 cells along the x-axis and 220 cells along the y-axis. The length of every cell along both x-axis and y-axis is $7.62\,m$. The layer thickness is 0.762 m. We suppose that the top boundary of the reservoir is at depth $1000\,m$.

For demonstrational purposes we apply local grid refinement (LGR) for a region of the reservoir (Fig. 1.1). The refinement is applied to the cells $i = 14, \ldots, 28$, $j = 66, \ldots, 90$. The index i is varying along x-axis while the index j is varying along y-axis. The number of cells is doubled along every axis in the region of refinement.

1.4. Input data

The input data for the simulation is a free formatted data file (RUN-file) which contains the description of the problem. The problem is described by keywords syntax. Every RUN-file is divided in the following sections:

The RUN-file sections		
RUNSPEC	-	In this section, general options and parameters of the simulation are specified;
GRID	-	In this section, the computational grid and the internal data structures are specified;

REGIONS	-	In this section, the petrophysical properties and the regions of the reservoir are specified;
PROPS	-	In this section, the thermophysical properties of the mixture and the host rock are specified;
INIT	-	In this section, the initial and the boundary conditions are specified;
SCHEDULE	-	In this section, the simulation schedule is specified.

The RUN-file

EXAMPLE-H2.RUN

```
1
2                    The MUFITS RUN-file for the example-H2
3                           (Release 2013.B)
4
5    Last updated on 25.05.2013.
6
7  ------------------------------------------------------------------------------
8
9    Note:
10   We type all comments in small letters while all keywords and mnemonics are
11      always in capital letters.
12
13 ------------------------------------------------------------------------------
14
15   Note:
16 -- any line beginning with '!' or '--' is a comment line;
17   any line not beginning with capital letter outside keyword
18 !  instruction is also a comment line.
19
20 ------------------------------------------------------------------------------
21
22   Note:
23   Any data line must be terminated by the slash '/' sign.
24
25 ------------------------------------------------------------------------------
26
27   Note:
28   We denote by the repeated symbols the following structural elements of this
29      RUN-file:
30      '###############' - delimits the sections of the RUN-file.
31      '<<<<<<<<<<<<<<<' - designates an opening bracket.
32      '>>>>>>>>>>>>>>>' - designates a closing bracket.
33      '^^^^^^^^^^^^^^^' - designates the keyword, which affects the order of the
34                          data input for all the following keywords (both in the
```

```
                          current and in the following sections).
      '==============' - merge the keywords and the comments in paragraphs.

--------------------------------------------------------------------------------


                           The section RUNSPEC begins
RUNSPEC   ###############################################################################
          In this section, the general options and parameters of the simulation
             are specified.
          We use two keywords: TITLE and PHYSICS in this section.

TITLE
   EXAMPLE-H2/
          We specify that all output file names will have the prefix EXAMPLE-H2.

PHYSICS
   SATCRT /
          The option SATCRT is recommended if the flow occurs under critical
             thermodynamic conditions.


                              The section GRID begins
GRID      ###############################################################################
          In this section, we must define the computational grid and the
             boundaries of the reservoir if we want to use the Dirichlet
             boundary conditions.

          Every new reservoir is specified within the brackets MAKE/ENDMAKE.
MAKE      <<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<
   CART 60 220 85 /
          The opening bracket MAKE has associated data, which define the type
             of the grid we want to use.
          CART data item designates that we want to use cartesian grid.
          60 220 85 data items designate that the grid has 60 cell along
             X-axis, 220 cell along Y-axis and 85 cells along Z-axis.

          ================================================================================

          The following 4 keywords are used for specification the geometrical
              properties of the reservoir and the grid blocks.

XYZBOUND
-- xmin-xmax   ymin-ymax     zmin-zmax
      2*          2*         1000.0 /
          The top boundary of the reservoir is at depth=1000 m.

DXV
```

```
   60*7.62 /
          Using the keyword DXV, we specify that the length of all 60 cells
             along x-axis is 7.62 meters.

DYV
   220*7.62 /
          Using the keyword DYV, we specify that the length of all 220 cells
             along y-axis is 7.62 meters.

DZV
   85*0.762 /
           Using the keyword DZV, we specify that the length of all 85 cells
             along z-axis is 0.762 meters.

          Note that father (when the following keyword ACTNUM is read) MUFITS
             automatically converts the cartesian grid to the corner point grid.

          ========================================================================

          The following keyword are used for setting active only the 50th
             layer of the reservoir. The cell activity is defined by the
             property ACTNUM. If ACTNUM=0 then the cell is inactive. If
             ACTNUM=1 then the cell is active. If ACTNUM=2 then the cell is
             active but its parameters are fixed, the parameters are not
             modified during the simulation. By default, all cells have the
             property ACTNUM=1.
          Firstly, we will make all cells inactive. We will set the property
             ACTNUM=0 for all cells. Secondly, we will make the 50th layer
             active. We will set the property ACTNUM=1 for all cells belonging
             to the 50th layer.

ACTNUM
   10000000*0 /
          The keyword ACTNUM can be used for specification the property ACTNUM
             for every cell. This keyword must be followed by the value of the
             property ACTNUM for every cell in the current input box. The input
             data order is defined by the ijk-indexes of the cells. The i-index
             is running in the first place, the j-index is running in the
             second place and the k-index running in the third place.
          Therefore, the keyword ACTNUM must be followed by the value 0 for
             every cell. The number of cells in the current input box is less
             than 10000000. Thus, simply typing '10000000*0' as the input data
             item we set the property ACTNUM to 0 in all cells.

BOX       ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
-- imin-imax jmin-jmax kmin-kmax
       2*        2*       50 50   /
          The input box defines a region of the grid based on the ijk-indexes
```

```
131             of the grid blocks. The region is i=[imin,imax], j=[jmin,jmax],
132             k=[kmin,kmax]. The input box affects the keywords used for the
133             properties input, like the keyword ACTNUM. By default,
134             the input box is positioned to the whole reservoir i=[1,60],
135             j=[1,220], k=[1,85]. The input box is modified by the keyword BOX.
136             Using this keyword we set the input box in a position when only
137             the 50th layer belong the box: i=[1,60], j=[1,220], k=[50,50].
138
139 ACTNUM
140    10000000*1 /
141           The keyword ACTNUM can be used for the property ACTNUM specification
142             only in the current input box. As the box is positioned to the 50th
143             layer we can simply type '10000000*1' as the input data item to
144             make the 50th layer active.
145
146 ENDBOX     ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
147           The keyword ENDBOX set the input box in the default position (the
148             reservoir). This keyword doesn't have associated data. After this
149             keyword is executed, the input box is in the position i=[1,60],
150             j=[1,220], k=[1,85].
151
152           ========================================================================
153
154           The following two keywords control the local grid refinement (LGR).
155             The LGR can be disabled by commenting out these two keywords.
156
157 CARFIN     ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
158 -- name   imin-imax   jmin-jmax   kmin-kmax   ni   nj   nk  parent_grid
159    LGR1    14   28     66   90       2*50     30   50   1  /
160           The LGRs of cartesian grid type are specified by the keyword CARFIN.
161             The LGR is specified by the ijk-indexes. The data associated with
162             this keyword are as follows:
163             item 1 (name) - the name of LGR. Father we can reference to the
164                LGR by its name 'LGR1';
165             items 2,3 (imin-imax) - the minimal and the maximal i-index of the
166                parent grid, to which the LGR is applied;
167             items 4,5 (jmin-jmax) - the minimal and the maximal j-index of the
168                parent grid, to which the LGR is applied;
169             items 6,7 (kmin-kmax) - the minimal and the maximal k-index of the
170                parent grid, to which the LGR is applied;
171             item 8 (ni) - the number of cells in the LGR along the
172                i-indexation axis (ni>imax-imin);
173             item 9 (nj) - the number of cells in the LGR along the
174                j-indexation axis (nj>jmax-jmin);
175             item 10 (nk) - the number of cells in the LGR along the
176                k-indexation axis (nk>kmax-kmin).
177
178 ENDFIN     ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
```

```
          After the keyword CARFIN is executed, MUFITS automatically creates
             the LGR and makes this grid active. The keyword ENDFIN makes the
             parent grid of the reservoir active. This keyword doesn't have
             associated data.
          The grid activity affect a lot of input data, e.g. the following
             keyword BOUNDARY, which is applied only to the cells nested in the
             active grid.

          ========================================================================

BOUNDARY
-- FLUXNUM   6 default    dire      5 default   option
--   ID       values      ction      values
     111      6*           J-         5*        INFTHIN /  -- left  boundary
     222      6*           J+         5*        INFTHIN /  -- right boundary
/
          We specify the left (y=0 m) and the right (y=1676.4 m) boundary of
             the reservoir by the keyword BOUNDARY. This keyword has associated
             data of the tabular form. The first data row describes the left
             boundary, the second data row describes the right boundary.
          Every row contains the following data items:
             item 1 - the boundary ID. For every boundary MUFITS automatically
                creates auxiliary cells, which are marked out by the property
                FLUXNUM=ID. By default, the property FLUXNUM=0;
             items 2-7 - imin,imax,jmin,jmax,kmin,kmax the region of the grid,
                for which the boundary is created;
             items 8-12 - the direction tags (I-,I+,J-,J+,K-,K+). This data
                items define the sides of the reservoir region, for which the
                auxiliary cells are created;
             item 13 - option. The record INFTHIN targets MUFITS to create
                infinitely thin boundary cells.
          Father the left boundary is marked out by the property FLUXNUM=111.
             The right boundary is marked out by the property FLUXNUM=222.

          ========================================================================

SAVEMVS
/
          The keyword SAVEMVS targets MUFITS to save the MVS-file for the
             grid defined within the current brackets MAKE/ENDMAKE. This
             keyword has the name of the file as the associated data. We use
             the default name of the file 'EXAMPLE-H2.MVS'.

ENDMAKE   >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>

                              The section REGIONS begins
REGIONS   ########################################################################
```

```
227          In this region, we must define petrophysical properties of the
228             reservoir and tune up the property ACTNUM property. Note
229             that the property ACTNUM can also be specified in the sections
230             INIT and SCHEDULE.
231
232 REGALL    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
233          The switch REGALL does not have associated data. This keyword targets
234             MUFITS to perform operations on array for all cells in the
235             simulation but not only for the cells in the current input box.
236             This keyword affects the data processing by the following keyword
237             EQUALREG, which is related to the auxiliary cells of the boundary
238             condition. It also affects the boundary conditions specification
239             in the section INIT.
240
241 EQUALREG
242 --           new
243 -- property value    marker    marker value
244 -- -------- -------- --------- ---------
245    ACTNUM   2        FLUXNUM   111      /
246    ACTNUM   2        FLUXNUM   222      /
247 -- -------- -------- --------- ---------
248 /
249          We must have the auxiliary cells created by MUFITS for the boundary
250             conditions under the fixed state conditions (the Dirichlet boundary
251             conditions). The parameters of these cells must not be modified
252             during the simulation. This behavior is engaged by setting the
253             property ACTNUM=2 for all auxiliary cells. The specification is
254             done by the keyword EQUALREG which has tabular associated data.
255             Every new row of the table engages a new data transformation. In
256             every row
257                item 1 - the mnemonic of the property, which is modified;
258                item 2 - the new value of the property;
259                item 3 - the marker property;
260                item 4 - the value of the marker property.
261             The EQUALREG operation can be described as follows: 'property' =
262                'new value' for all cells, which have the property 'marker'
263                 equal to the 'marker value'.
264
265          ============================================================================
266
267          In this paragraph, we load the petrophysical properties from files.
268
269 LOADING   ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
270    IJK /
271          The keyword LOADING affects the following keywords PORO, PERMI, PERMJ,
272             PERMK. This keyword has one associated data item. The mnemonic IJK
273             targets MUFITS to load data from files according to ijk-indexation
274             in the current input box. MUFITS assumes that every loaded file
```

```
            contains the values of the properties (PORO, PERMI, PERMJ, PERMK)
            for every cell in the current input box. The values are ordered
            in that i-index is running in the 1st place, j-index is running
            in the 2nd place, k-index is running in the 3rd third place.

POROMIN
   0.01 /
         The keyword POROMIN targets MUFITS to increase all the properties
            PORO to the value 0.01 if they are below this value. By the default
            option, the minimal porosity is 0.001. This option eliminates the
            cells with small pore volume from the simulation and consequently
            makes the simulation more stable.

PORO
   ASCII '../EXAMPLE-H2.PORO'  /
         The keyword PORO can be tuned up to load the porosity from an include
            file. If the 1st data item of this keyword is the mnemonic ASCII
            or BINARY then the loading is invoked. In this case, the 2nd data
            item is file name, from which the porosity is loaded. The mnemonic
            ASCII signifies that the porosity file is a formatted file. The
            mnemonic BINARY signifies that the the porosity file is a binary
            file.
         According to the earlier specification of the arrays loading mode
            (the keyword LOADING), the file EXAMPLE-H2.PORO must contain
            the porosity value for every cell of the reservoir. The values are
            ordered in that i-index is running in the 1st place, j-index
            is running in the 2nd place, k-index is running in the 3rd
            place.

PERMI
   ASCII '../EXAMPLE-H2.PERMX' /
         The syntax of the keyword PERMI is identical to the syntax of the
            keyword PORO except that the keyword is for loading the x-direction
            permeabilities. The permeability dimension is mD (millidarcy).

PERMJ
   ASCII '../EXAMPLE-H2.PERMY' /
         The syntax of the keyword PERMJ is identical to the syntax of the
            keyword PORO except that the keyword is for loading the y-direction
            permeabilities. The permeability dimension is mD (millidarcy).

PERMK
   ASCII '../EXAMPLE-H2.PERMZ' /
         The syntax of the keyword PERMK is identical to the syntax of the
            keyword PORO except that the keyword is for loading the z-direction
            permeabilities. The permeability dimension is mD (millidarcy).

         ================================================================
```

```
323
324 RPTRES
325    MPINUM XCOORD YCOORD DEPTH PORO PERMI PERMJ PERMK  /
326           We specify the properties we want to save in the file
327              'EXAMPLE-H2.GRID.SUM' after the section REGIONS. The file will
328              contain the properties MPINUM, XCOORD, etc.
329
330 SAVERES
331    /
332           Using the keyword SAVERES we target MUFITS to save
333              'EXAMPLE-H2.GRID.SUM' file after the section REGIONS.
334              We do not want to change the name of the summary file. That's why
335              we do not modify the default data item 'EXAMPLE-H2.GRID.SUM'
336              of the keyword SAVERES.
337
338                              The section PROPS begins
339 PROPS      ######################################################################
340           In this section, we must define the thermophysical properties of
341              binary mixture, host rock as well as the relative permeability
342              curves.
343
344 LOADEOS
345    '../../INCLUDE/CO2H2O_V3.0.EOS' /
346           The keyword LOADEOS is used for loading the mixture properties from
347              the EOS-file. This keyword has as associated data the system path
348              to the file.
349
350           The rock properties for every region ROCKNUM are specified within
351              the brackets ROCK/ENDROCK.
352 ROCK       <<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<
353    0 /
354           The opening bracket ROCK has one associated data item, which is the
355              ROCKNUM region ID. By default, all cells belong to the region
356              ROCKNUM=0. Therefore, we set the data item to 0.
357
358 RMODEL1
359 -- grain density               heat capacity
360 --  [kg/m^3]                    [kJ/kg/K]
361       2500         4*              1.0    /
362           The easiest way for the rock properties specification is by using the
363              keyword RMODEL1.
364           The first data item associated with this keyword is the host rock
365              density.
366           The record 4* means that we leave the default values for the data
367              items 2-5.
368           The 6th data item associated with the keyword is the host rock heat
369              capacity.
370
```

```
ENDROCK    >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>

           The relative permeabilities for every region SATNUM are specified
              within the brackets SAT/ENDSAT.
SAT        <<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<
   0 /
           The opening bracket SAT has one associated data item, which is the
              SATNUM region ID. By default, all cells belong to the region
              SATNUM=0. Therefore, we set the data item to 0.

SATTAB
--  sH2O     krH2O      krCO2
    0.2     0.000000   1.000000 /
    0.3     0.000316   0.737758 /   The  Brooks and Corey curves
    0.4     0.005056   0.499535 /
    0.5     0.025600   0.302400 /      Sl_min=0.2
    0.6     0.080908   0.155832 /      Sg_min=0.05
    0.7     0.197530   0.061728 /
    0.8     0.409600   0.014400 /
    0.9     0.758834   0.000572 /
    0.95    1.000000   0.000000 /
/
           The keyword SATTAB is followed by the tabular data for the relative
              permeabilites.
              The 1st column is the liquid phase saturation, which is water
              (sH2O). The 2nd column is the liquid phase relative
              permeability (krH2O). The 3rd column is the gaseous phase
              relative permeability, which is the relative permeability
              of supercritical CO2 phase.

ENDSAT     >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>

PHASES
-- name     pres    enth    composition
--          [MPa] [kJ/mol]  CO2     H2O
   LH2O     1.0      5.0    0.0     1.0  /        - H2O rich phase
   SCO2     10.0    10.0    1.0     0.0  /        - CO2 rich phase
/
           The keyword PHASES defines new MNEMONICS for data output. This keyword
              is followed by tabular data and every line of these data defines an
              individual phase. The 1st column is the phase name (not more
              than 4 characters). The following data items define typical
              thermodynamic parameters of the phase. The 2nd column is
              pressure, the 3rd is the enthalpy, the 4th and 5th are the molar
              composition of binary mixture.
           We define two phases. The 1st is the liquid water (LH2O). The 2nd is
              the supercritical CO2 phase.
```

```
                          The section INIT begins
INIT      ###########################################################################
          In this section, we must define the initial and boundary conditions.
             We must define the required number of parameters for every cell
             associated with the simulation.

OPERAREG
-- modified argument           marker    opera    paramet  paramet  paramet
-- property property marker    value       tion      er1      er2      er3
-- -------- -------- --------- --------- -------- -------- -------- ---------
   PRESSURE YCOORD   FLUXNUM   0         MULTA    7.5     -1.789549034E-3 /
-- -------- -------- --------- --------- -------- -------- -------- ---------
/
          It is easy to calculate that if pressure is 7.5 MPa at the boundary
             y=0 m, and pressure 4.5 MPa at the boundary y=1676.4 m then the
             pressure distribution must be the following function:

                 PRESSURE=7.5-1.789E-3*YCOORD    [MPa]

          To specify this distribution of pressure we use the keyword OPERAREG.
             This keyword has tabular associated data. The keyword data items
             are as follows:
             item 1 - the modified property mnemonic;
             item 2 - the argument property mnemonic;
             item 3 - the marker mnemonic;
             item 4 - the marker value;
             item 5 - the data transformation mnemonic. This argument specifies,
                which operation is applied to the data;
             items 6-8 - the parameters of the operation.
          If the operation is MULTA then MUFITS do the following:

              'modified property'='parameter1'+'parameter2'*'argument property'
              for all cells marked out as 'marker' is equal to 'marker value'.

EQUALREG
-- -------- -------- --------- ---------
   COMP1T   0.0      FLUXNUM   0         /
   TEMP     295.15                       /
-- -------- -------- --------- ---------
   PRESSURE 4.5      FLUXNUM   222       /
   COMP1T   0.0                          /
   TEMP     295.15                       /
-- -------- -------- --------- ---------
   PRESSURE 7.5      FLUXNUM   111       /
   COMP1T   1.0                          /
   TEMP     320.15                       /
-- -------- -------- --------- ---------
/
```

```
          The other initial condition except the conditions for pressure as well
             as the boundary conditions are specified by the keyword EQUALREG.
             We specify that:
             data row 1 - the reservoir is initially saturated by pure H2O;
             data row 2 - the initial reservoir temperature is 295.15 K;
             data row 3 - the pressure at the right boundary (y=1676.4 m)
                is 4.5 MPa;
             data row 4 - there is pure H2O at the right boundary;
             data row 5 - the temperature at the right boundary is
                295.15 K;
             data row 6 - the pressure at the left boundary (y=0 m) is 7.5 MPa;
             data row 7 - pure CO2 is injected through the left boundary;
             data row 8 - the temperature of the injected CO2 is 320.15 K.
          Note that the numbers 111 and 222 are the boundary markers, which
             are specified by the keyword BOUNDARY in the section GRID.

          ================== output specification ============================

RPTSOL
   PHST PRES TEMP SAT#LH2O SAT#SCO2 COMP1T /
           The properties, which we want to save in summary files during the
              simulation, can be specified using the keyword RPTSOL.
           We want to save the properties DEPTH, PHST, PRES etc.
           Note that SAT#LH2O is the saturation of the phase LH2O which was
              defined using keyword PHASES in the section PROPS.
           Note that the keyword RPTSOL has an arbitrary number (up to 10000)
              of associated data items. The data items are the property
              mnemonics. The mnemonics with the special meaning are as follows:
                 CLEAN - targets MUFITS to delete all data items in the list
                    RPTSOL;
                 INSERT - the subsequent mnemonics are added to the list RPTSOL
                   (default option);
                 DELETE - the subsequent mnemonics are deleted from the list
                    RPTSOL.
           The input of the same type is for the keywords RPTGRID, PHYSICS and
              REPORTS in this RUN-file.

                           The section SCHEDULE begins
SCHEDULE   ##########################################################################

REPORTS
   CLEAN MATBAL CONV LINSOL /
           The keyword REPORTS defines the reports outputted in the LOG-file.
           The 1st record CLEAN means that we clean the default list of
              outputted reports.
           We enable the output of the material balance reports (MATBAL), the
              convergence reports (CONV) and the linear solver reports (LINSOL).

```

```
TUNING
-- linear solver setup:
--        ilut_fill             maxiter        Krylov_space
    34*      1.0         5*      300               150  /
           The linear solver tuning can be done by the keyword TUNING. By
              the default option MUFITS uses the linear solver GMRES and the
              preconditioner ILUT. The data items related to the linear solver
              are:
                 item 35 - the ILUT 'fill' parameter;
                 item 41 - the maximal number of the linear solver iterations;
                 item 42 - the number of iterations between GMRES restarts (the
                    dimension of the Krylov space).

TUNING
-- timestep setup
-- limit   max    next   min
    1      31     10      /
           The timestep control can be tuned up using the keyword TUNING. The
              data items related to the timestep control are:
                 item 1 - the timestep limit [days]. The next timestep can't
                    be greater than this value;
                 item 2 - the maximal timestep [days];
                 item 3 - the explicitly specified next timestep [days];
                 item 4 - the minimal timestep [days].

           ========================================================================

TSTEP
   50*365.25 /
           By the keyword TSTEP we define the time of output. The year duration
              in days is estimated as 365.25 days. We want to simulate the flow
              over 50 years and save the simulation results after every
              year in the simulation schedule. This behavior is specified by
              the argument '50*365.25'. Thus, the output will be saved in the
              summary files at times: 365.25, 730.50, 1095.75, etc. days.
           When the simulator comes to this record TSTEP in the RUN-file
              it performs simulation and produces output for the described
              times.

                The section SCHEDULE must be terminated by the keyword END
END        ########################################################################

MUFITS does not read the following records.
```

Every section has its own list of available keywords.

Farther we suppose that the RUN-file for this exercise is EXAMPLE-H2.RUN. See the comments in this file for better understanding of how the data file is prepared.

1.5. How to run the simulation

You must have MPICH installation on your system for running MUFITS simulations.

A sequence of action for running the simulation on Windows system is given below:

1. create the folder SIMULATIONS (for example on disk D). Navigate to the folder SIMULATIONS;
2. create the folder BIN in the folder SIMULATIONS;
3. copy the simulator executable H32.EXE to the folder BIN;
4. create the folder INCLUDE in the folder SIMULATIONS;
5. copy the mixture properties file CO2H2O_V3.0.EOS to the folder INCLUDE;
6. create the folder EXAMPLE-H2 in the folder SIMULATIONS. Navigate to the folder EXAMPLE-H2;
7. copy the files EXAMPLE-H2.PORO, EXAMPLE-H2.PERMX, EXAMPLE-H2.PERMY, EXAMPLE-H2.PERMZ to the folder EXAMPLE-H2;
8. create the folder SIM1 in the folder EXAMPLE-H2 ;
9. copy the file EXAMPLE-H2.RUN to the folder SIM1;

10. navigate to the folder 1;
11. create the text file EXAMPLE-H2.BAT in the folder SIM1;
12. type the following command in the file EXAMPLE-H2.BAT: "C:/Program Files (x86)/MPICH2/bin/mpiexec.exe" -n 2 ../../BIN/H32.EXE EXAMPLE-H2.RUN > EXAMPLE-H2.LOG. Here "C:/Program Files (x86)/MPICH2/bin/mpiexec.exe" is the system path to your installation of MPICH. You must modify this record according to the installation of MPICH on your system. The record '-n 2' defines that 2 processes granted to the simulation. You must modify the number after '-n' if you want to modify the number of processes. Save and close the file EXAMPLE-H2.BAT;
13. execute the file EXAMPLE-H2.BAT (double click on this file).

1.6. Output data

The following files are created by MUFITS in the directory SIMULATIONS/EXAMPLE-H2/s1 after the successful simulation:

Output files		
EXAMPLE-H2.LOG	-	the simulation LOG-file;
EXAMPLE-H2.MVS	-	the MVS-file for the considered problem;
EXAMPLE-H2.GRID.SUM	-	the SUM-file saved after the section REGIONS;
EXAMPLE-H2.0000.SUM, EXAMPLE-H2.0001.SUM,..., EXAMPLE-H2.0050.SUM	-	the SUM-files for different times in the simulation schedule.

1.7. Simulation results

The videos containing the simulation results can be found at [2, 3]

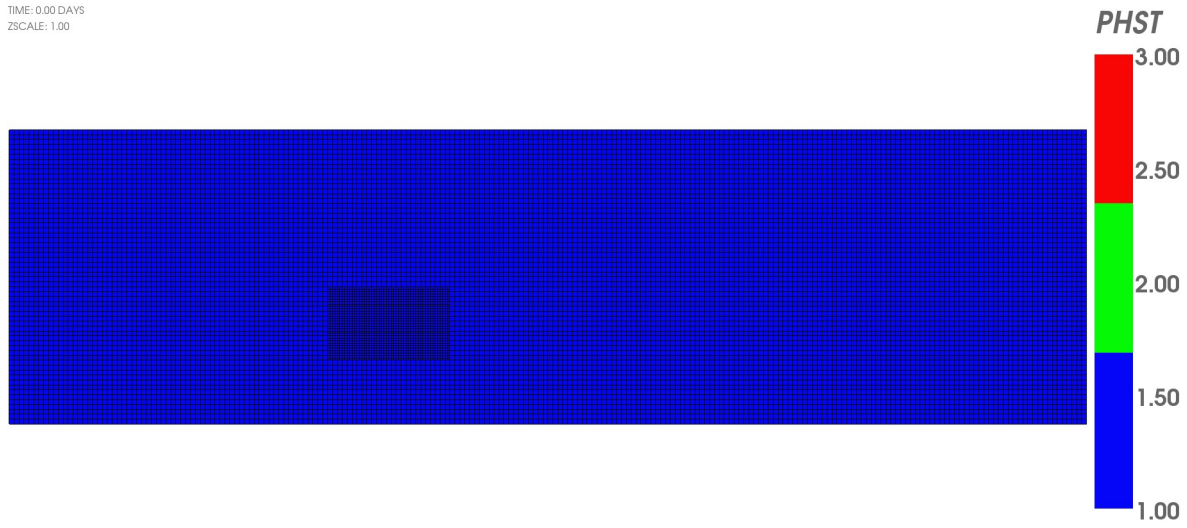

Figure 1.2: The number of phases at $t = 0$ years

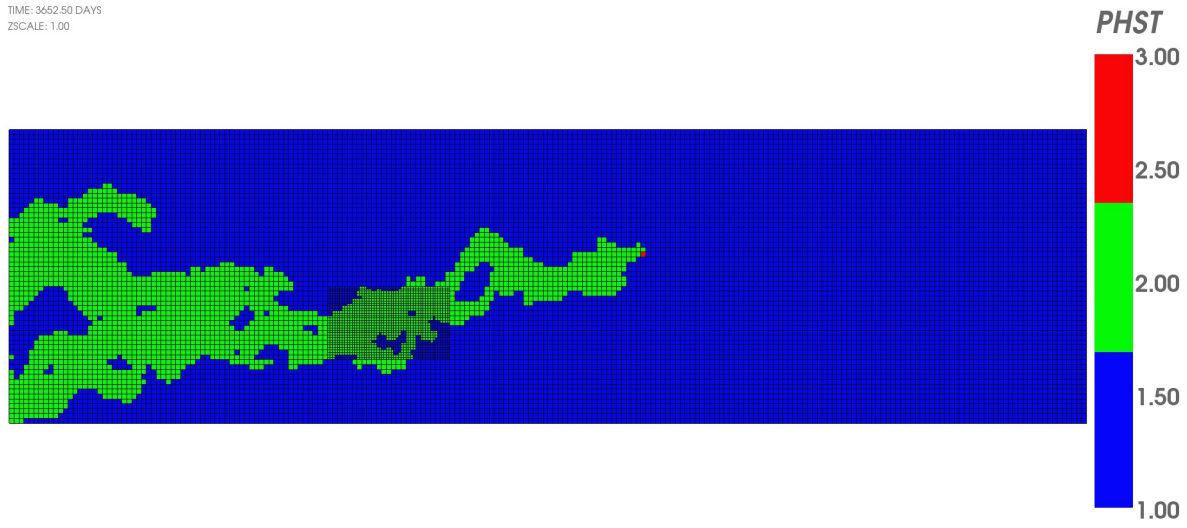

Figure 1.3: The number of phases at $t = 10$ years

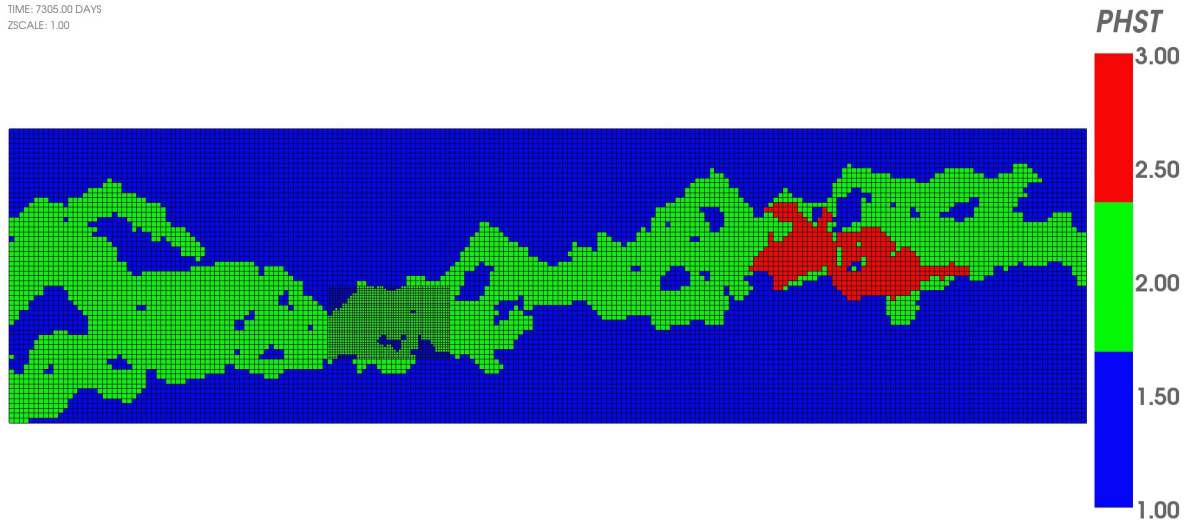

Figure 1.4: The number of phases at $t = 20$ years

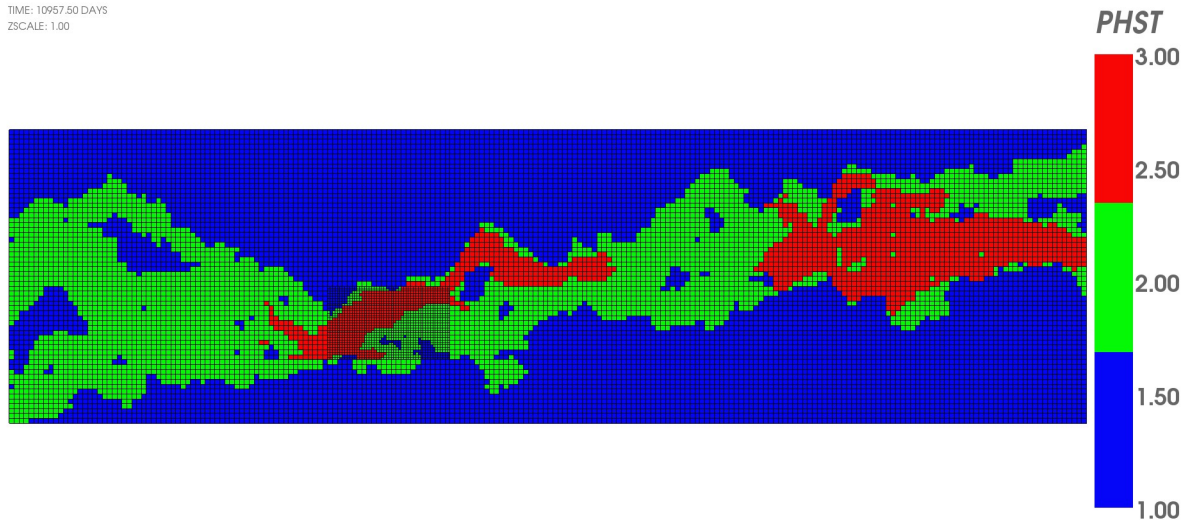

Figure 1.5: The number of phases at $t = 30$ years

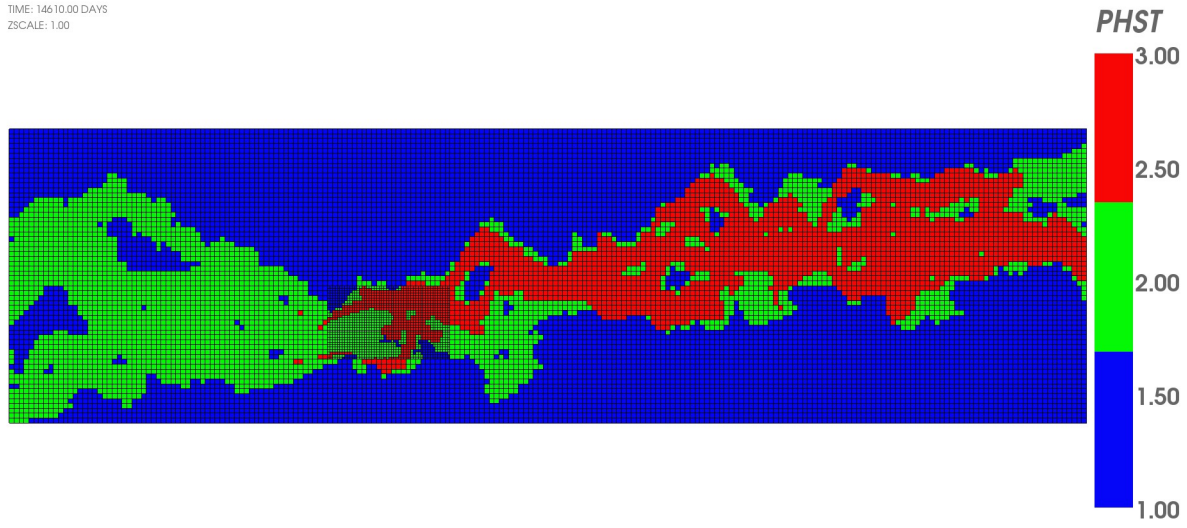

Figure 1.6: The number of phases at $t = 40$ years

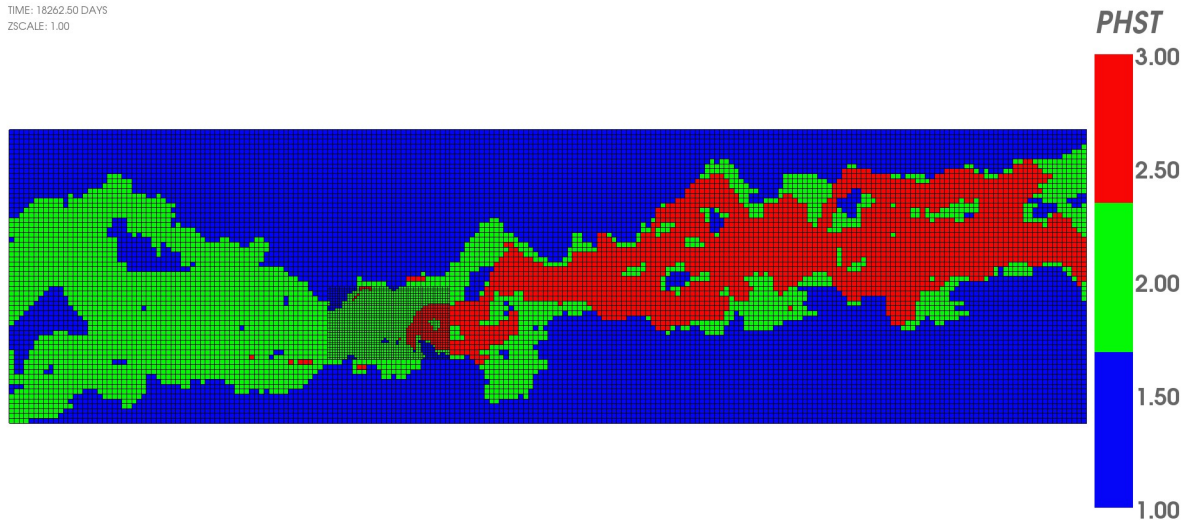

Figure 1.7: The number of phases at $t = 50$ years

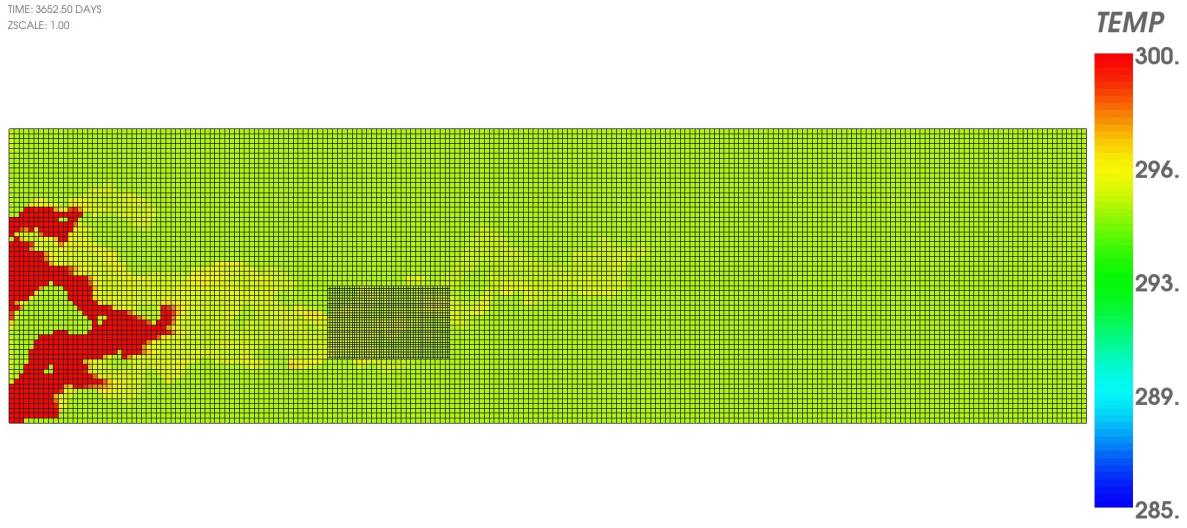

Figure 1.8: The temperature at $t = 10$ years

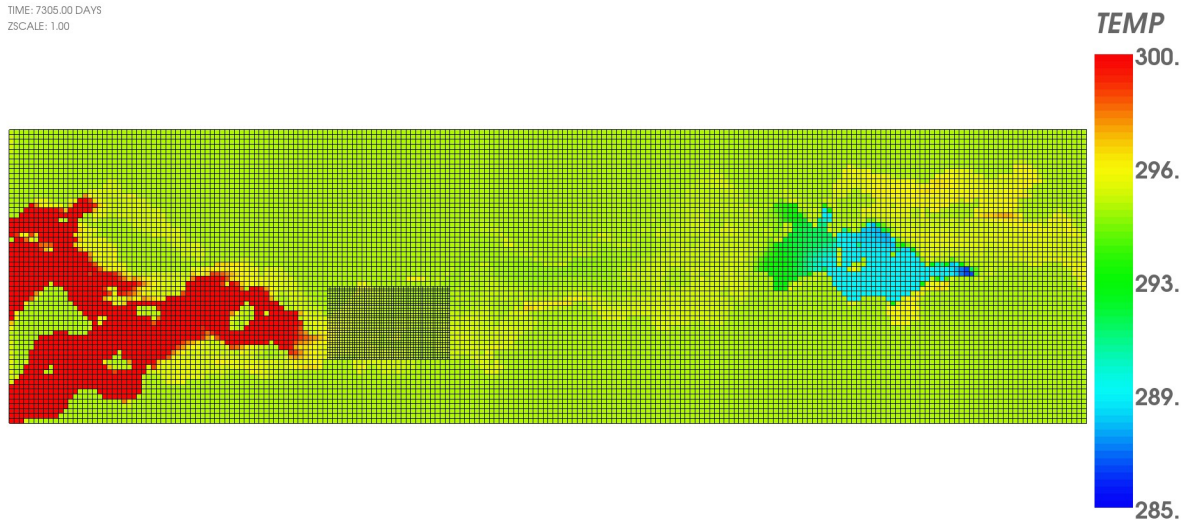

Figure 1.9: The temperature at $t = 20$ years

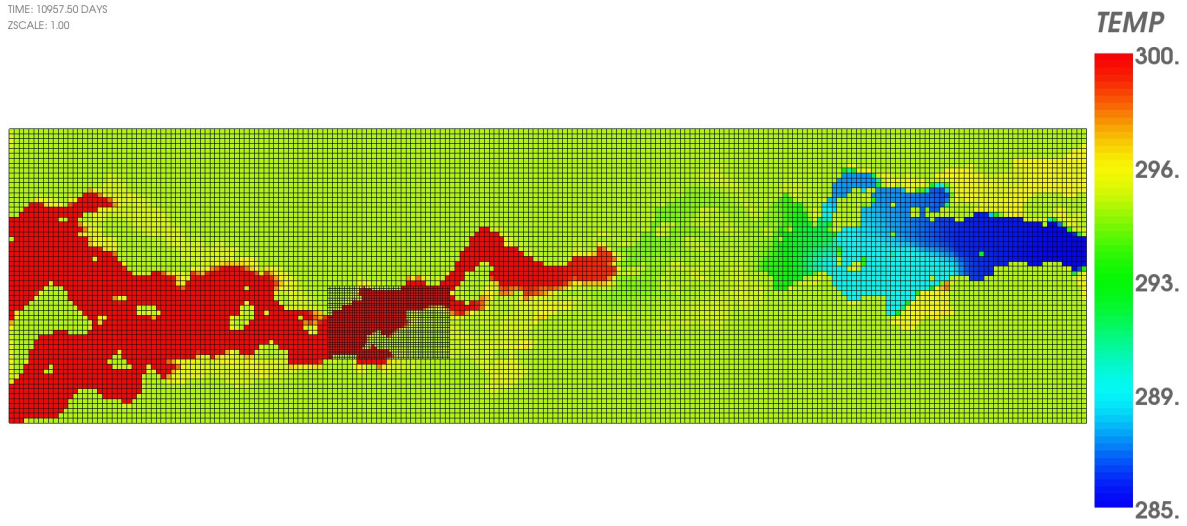

Figure 1.10: The temperature at $t = 30$ years

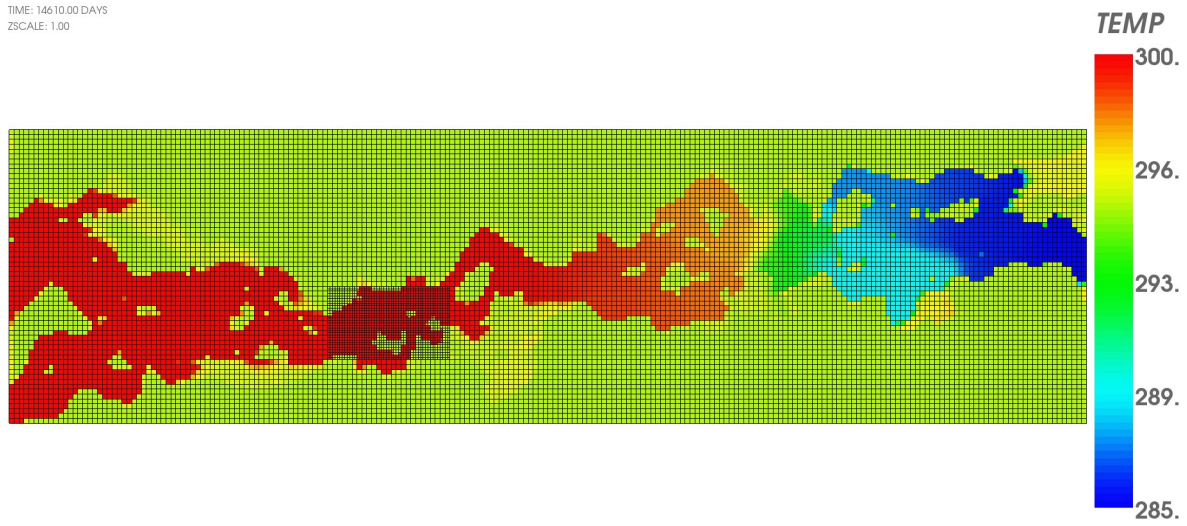

Figure 1.11: The temperature at $t = 40$ years

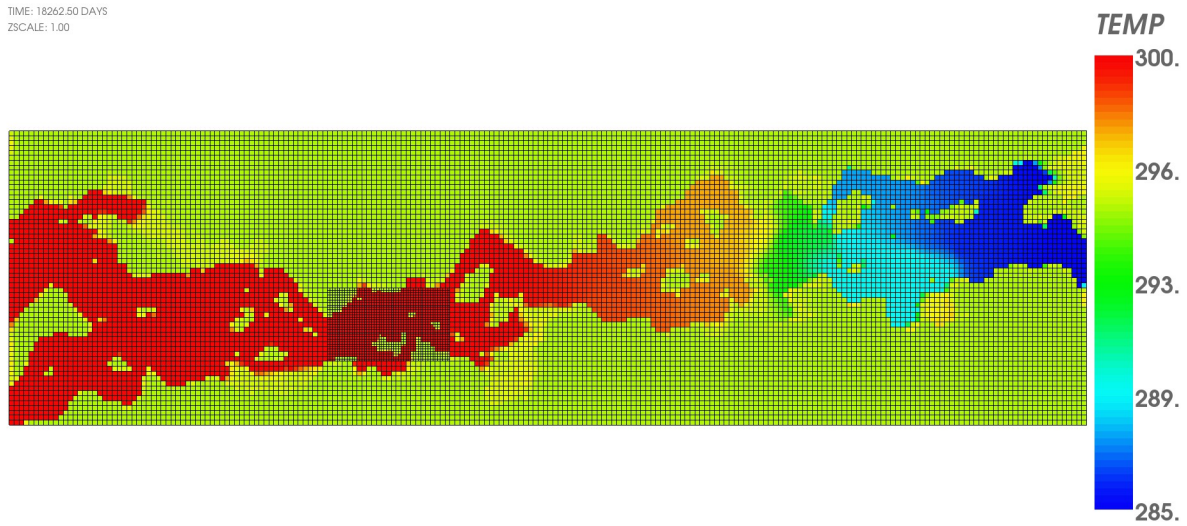

Figure 1.12: The temperature at $t = 50$ years

References

1. The 10th SPE dataset. http://www.spe.org/web/csp.

2. *Afanasyev, A.A.* Multiphase compositional modelling of CO_2 injection under subcritical conditions: The impact of dissolution and phase transitions between liquid and gaseous CO_2 on reservoir temperature. Int. J. Greenhouse Gas Control (2013), http://dx.doi.org/10.1016/j.ijggc.2013.01.042.

3. MUFITS simulator website. http://www.mufits.imec.msu.ru.