MUFITS

Multiphase Filtration Transport Simulator
version 2013.B

Example-H4

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1 Example-H4

1.1. Introduction

The example-H4 concerns simulation of CO_2 injection in the Johansen formation using a real-scale geological model of the formation. We use the "'sector model with heterogeneous rock properties"', which can be downloaded at [1]. The computational grid is shown in Fig.1.1. The lateral extensions of the domain are up to 100 km. The model comprises 11 layers of grid blocks. There are 5 vertical faults in the model. We simulate two scenarios of CO_2 injection in this formation for two different locations of the injection well in the region of depression.

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

- conduct a 3D simulation using corner-point grid;
- specify the permeability ratio;
- specify multiple faults using an include file;
- apply multiple local grid refinements as well as the nested refinements;
- approximate the injection well using the point sources;
- initiate the automatic fluid-in-place calculation.

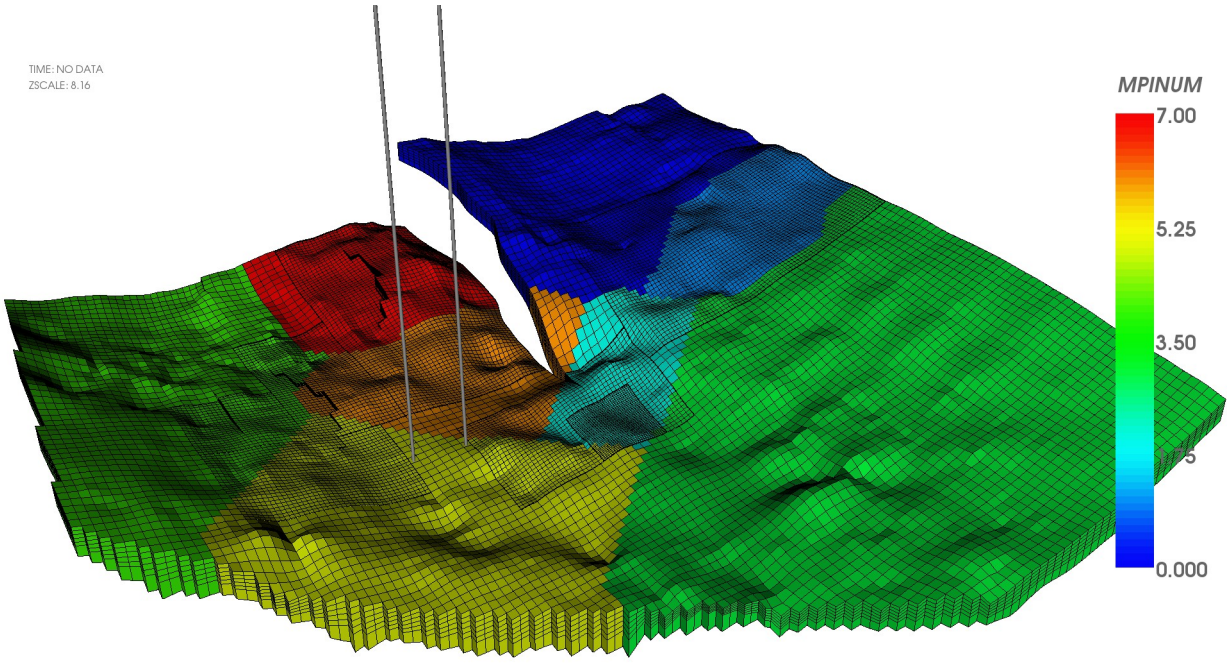

Figure 1.1: The computational grid, an example of the domain decomposition for 8 nodes and the location of the injection well for the two injection scenarios.

1.2. The problem formulation

The domain $100 \times 100 \times 11$ grid blocks comprises 9 layers all representing the high permeable sandstones in the Johansen formation. The top 5 layers represent a shale (caprock) above the formation. The layers 6 - 10 are the high-permeablilty layers representing the sandstones of the Johansen formation. The layer 11 is the low-permeability shale. There are 5 faults in the model. The transmissibility multiplier for all faults is 0.1.

The initial pressure is 31.31 MPa whereas the initial temperature is $100°C$ at the reference depth 3100 m [1]. The geothermal gradient is $3°C$ per 100 m. The top and the bottom boundaries of the reservoir are impermeable and fully insulated. The pressure and the temperature at the lateral boundaries of the domain and at the fault plane are constant and are equal to the initial parameters before injection.

We consider two injection scenarios for two different coordinates of the injection well (Fig.1.1). The well INJ1 location is the same as in [2]. The well INJ2 is shifted with respect to the well INJ1 for approximately 3 km to the west. We suppose that both wells are perforated only in the layers 6, 7 and 10 because the layers 8, 9 around the well INJ2 represent a low-permeability wedge. The i- and j-indexes of the grid blocks, in which the well is perforated as well as the well coordinates are provided below.

For both injection scenarios, we simulate the injection of 400 Mt of CO_2 over 100 years. Therefore, the constant injection rate 4 $Mt/year$ is consistent with [2]. After the injection is shut down, we continue the simulation over 2500 years to evaluate the preferable directions of CO_2 migration. The total simulation time is 2600 years.

The parameters of the problem are summarized below:

The parameters of the problem		
Domain	-	Specified in the file NPD5.grdecl. The domain comprises $100 \times 100 \times 11$ cells;
Porosity	-	Specified in the file NPD5_Porosity.txt;
Permeability	-	Specified in the file NPD5_Permeability.txt. The permeability is isotropic in the lateral extensions. The permeability ratio is 0.1 (the vertical permeability is ten times less than the horizontal permeability);
Faults	-	Specified in the file NPD5_Faults.txt;
Transmissibility multiplier for the faults	-	0.1;
Rock grain density	-	2500 kg/m^3;
Rock heat capacity	-	1 $kJ/kg/K$;
Rock compressibility	-	0;

Relative permeability	-	Tabular data. The data were prepared using the files Scaled_RelPermWater.txt and Scaled_RelPermCO2.txt, which can be downloaded at [1].
Water critical saturation	-	0.1;
CO_2 critical saturation	-	0.2;
Capillary pressure	-	neglected;
Heat conduction	-	neglected;
Initial reservoir pressure	-	31.31 MPa at the reference depth 3100 m;
Initial reservoir temperature	-	373.15 K at the reference depth 3100 m;
Geothermal gradient	-	3 K per 100 m;
Initial composition	-	The reservoir is saturated by pure water;
The top and the bottom boundaries of the domain	-	Impermeable and fully insulated;
The lateral boundaries	-	The open boundaries. The parameters at this boundaries are equal to the initial parameters in the reservoir before injection;
Injection coordinates	-	The well INJ1: $i = 58$, $j = 48$; The well INJ2: $i = 64$, $j = 44$. Both wells are perforated in the layers 6,7,10;
Injection rate	-	10951.4031 t/day;
Injected mixture parameters	-	Pure CO_2 is injected. The temperature is 353 K under 25 MPa;
Duration of the injection period	-	100 years;
Duration of the post-injection period	-	2500 years.

1.3. Input data

The input data for the simulation is a free formatted data file (the RUN-file), which contains the description of the problem. The problem is described by the keywords. Farther we suppose that the RUN-file for this exercise is EXAMPLE-H4.RUN. Review the comments in this file for better understanding of how the data file is prepared.

Initial conditions

At the present time MUFITS doesn't support the reservoir equilibration option. Therefore, the initial distribution of pressure and the temperature are specified by the explicit relations:

$$P = 0.31 + 0.01z \ [MPa] \tag{1.1}$$

$$T = 283 + 0.03z \ [K] \tag{1.2}$$

Here, P is the pressure (the property PRES), T is the temperature (the property TEMP), z is the depth (the property DEPTH). According to (1.1), (1.2), the pressure is equal to 31.31 MPa and the temperature is equal to 373 K at the reference depth 3100 m. Thus, the initial distribution is consistent with the problem formulation.

In the relation (1.1), we suppose that the water density is 1000 kg/m^3 under the reservoir conditions. This is only an approximation because the water density depends on the temperature as well as on the pressure. Therefore, the pressure distribution (1.1) is only an estimation of the initial hydrostatic equilibrium in the reservoir. In order to evaluate a more realistic hydrostatic equilibrium we conduct a pre-injection simulation over 1 year. During this simulation the pressure line up with hydrostatic distribution consistent with the temperature distribution in the reservoir. Thus, the simulation schedule looks as follows:

The simulation schedule		
0-1 years	-	The pre-injection period. The hydrostatic equilibrium evaluation;
1-101 years	-	The period of injection;
101-2601 years	-	The post-injection period.

Injection well

We consider two injection scenarios for two different locations of the injection well. The coordinates of the wells are provided in the table below.

The injection well coordinates				
Well	x $[m]$	y $[m]$	i-index	j-index
INJ1	523737	6692500	58	48
INJ2	520837	6693333	64	47

At the present time MUFITS doesn't support the well option for coupled simulations of flows both in the reservoir interior and in the wellbore. Therefore, we approximate the injection wells INJ1 and INJ2 by three point sources. The x and y coordinates of the point sources are equal to the coordinates of the injection well. The sources are located in the layers 6, 7 and 10 of the domain (a source in every layer). The injection rate for every source is 1.333 $Mt/year$, thus the overall injection rate is 4 $Mt/year$. The point sources approximate the injection well if the injection rates are equal for all perforations.

Relative permeabilities

The relative permabilties are specified in tabular form. The data were prepared using the files Scaled_RelPermWater.txt and Scaled_RelPermCO2.txt, which can be downloaded at [1]. The first column in the table below is the water saturation, the second column is the water relative permeability, the third column is the CO_2 phase relative permeability.

Relative permeabilities

```
0.100   0.0000  0.4284
0.150   0.0020  0.3800
0.204   0.0084  0.3292
0.258   0.0281  0.2820
0.313   0.0592  0.2382
0.367   0.1017  0.1978
0.421   0.1555  0.1610
```

```
    0.475   0.2206  0.1276
    0.529   0.2971  0.0976
    0.583   0.3850  0.0712
    0.638   0.4842  0.0482
    0.692   0.5948  0.0286
    0.746   0.7167  0.0126
    0.800   0.8500  0.0000
```

Local grid refinements

We apply 7 local grid refinements for better resolution of the CO2 plume spreading along the caprock as well as for the simulator capabilities demonstration. The regions of the domain, to which the refinement is applied, can be seen in Fig.1.1 Following [2], we double the number of grid blocks in the x and y directions and quadruple the number of blocks in the vertical direction. The refinement is applied to the lowest layer of the caprock and to the upper three layers of the formation (layers 5 - 8). We use a nested refinement LGR2A for demonstrational purposes.

The parameters of the refinements are provided below

The local grid refinements		
Name	ijk-box to which the refinement is applied	Parent grid
LGR1	$i = [62, 72]$, $j = [17, 39]$, $k = [5, 8]$	-
LGR2	$i = [36, 57]$, $j = [45, 60]$, $k = [5, 8]$	-
LGR3	$i = [1, 35]$, $j = [25, 50]$, $k = [5, 8]$	-
LGR4	$i = [44, 61]$, $j = [1, 39]$, $k = [5, 8]$	-
LGR5	$i = [65, 84]$, $j = [40, 52]$, $k = [5, 8]$	-
LGR6	$i = [73, 84]$, $j = [29, 39]$, $k = [5, 8]$	-
LGR2A	$i = [8, 23]$, $j = [15, 32]$, $k = [3, 11]$	LGR2

The RUN-file

EXAMPLE-H4.RUN

```

                The MUFITS RUN-file for the example-H4
                       (Release 2013.B)

```

```
   Last updated on 25.05.2013.

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

   Note:
   We type all comments in small letters while all keywords and mnemonics are
      always in capital letters.

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

   Note:
-- any line beginning with '!' or '--' is a comment line;
   any line not beginning with capital letter outside keyword
!  instruction is also a comment line.

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

   Note:
   Any data line must be terminated by the slash '/' sign.

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

   Note:
   We denote by the repeated symbols the following structural elements of this
      RUN-file:
      '###############' - delimits the sections of the RUN-file.
      '<<<<<<<<<<<<<<' - designates an opening bracket.
      '>>>>>>>>>>>>>>' - designates a closing bracket.
      '^^^^^^^^^^^^^^' - designates the keyword, which affects the order of the
                         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 sataset description:

        This is MUFITS RUN-file for the NPD5 model of the Johansen formation.

        Data sets used:
                Grid            NPD5.grdecl
                Faults          NPD5_Faults.txt
                Porosity        NPD5_Porosity.txt
                Permeability    NPD5_Permeability.txt
                Rel. Perm.      Scaled_RelPermWater.txt & Scaled_RelPermCO2.txt

        All files can be loaded at:
              http://www.sintef.no/Projectweb/MatMoRA/Downloads/Johansen/
```

```
              "A sector model with heterogeneous rock properties" (NPD5 model)

        The geological model has 11 layers:
              layers 1-5   -  caprock, shale above Johansen;
              layers 6-10  -  high permeable layers (Johansen formation);
              layers 11    -  shale.

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

                          The section RUNSPEC begins
RUNSPEC   ###############################################################################
          In this section, the general options and parameters of the simulation
             are specified.

TITLE
   EXAMPLE-H4 /
          We specify that all output file names will have the prefix EXAMPLE-H4.

                          The section GRID begins
GRID      ###############################################################################
          In this section, we must define the geometrical and logical structures
             of the reservoir (computational grid, boundaries, faults, sources,
             etc.).

          Every new reservoir is specified within the brackets MAKE/ENDMAKE.
MAKE      <<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<
   CORNER 100 100 11 /
          The opening bracket MAKE has the following associated data:
             item 1 - the grid type mnemonic:
                CART   - cartresian grid;
                CORNER - corner-point grid (default option);
                RADIAL - radial grid;
             item 2 - the number of cells along the i-indexation axis (x-axis);
             item 3 - the number of cells along the j-indexation axis (y-axis);
             item 4 - the number of cells along the k-indexation axis (z-axis).

IDTOMPI
   1  1  11 /
          The keyword IDTOMPI is used for tuning the domain decomposition. This
             keyword allows to merge the grid cells in groups that cannot be
             distributed among different processes in parallel simulation. Thus
             cells belonging to the same group also belong to the same process.
             The groups are build on basis of the ijk-indexation. The group is
             a box in the ijk-indexation basis. The keyword IDTOMPI has 3
             associated arguments:
                item 1 - the number of cells along the i-indexation axis
                   (x-axis in cartesian grid), which form a group;
                item 2 - the number of cells along the j-indexation axis
```

```
                  (y-axis in cartesian grid), which form a group;
               item 3 - the number of cells along the k-indexation axis
                  (z-axis in cartesian grid), which form a group.
         In full-scale simulations, which use very thin cells, connections
            along z-axis shared by different processes in parallel simulation
            are not recommended. This can be done by setting the 3rd argument
            associated with the keyword IDTOMPI to the number of cells along
            z-axis in the grid, which in this simulation is 11.

INCLUDE
   '../NPD5.grdecl' /
         The formatted corner-point grid file (the file extension
            .GRDECL) is loaded using the keyword INCLUDE. The asscociated
            data of this keyword is the system path to the grid file. MUFITS
            recognizes the usual keywords in the file like: COORD, ZCORN,
            ACTNUM, SPECGRID (the 1st three data items must be the same as
            specified by the keyword MAKE; is used for the grid dimension
            checking), MAPAXES, MAPUNITS (must be METRES), GRIDUNITS
            (must be METRES).

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

CARFIN    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
-- name   imin-imax   jmin-jmax   kmin-kmax   ni   nj   nk  parent_grid
   LGR1    62   72     17   39     5    8     22   46   16 /
CARFIN    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
   LGR2    36   57     45   60     5    8     44   32   16 /
CARFIN    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
   LGR3    1    35     25   50     5    8     70   52   16 /
CARFIN    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
   LGR4    44   61     1    39     5    8     36   78   16 /
CARFIN    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
   LGR5    65   84     40   52     5    8     40   26   16 /
CARFIN    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
   LGR6    73   84     29   39     5    8     24   22   16 /
CARFIN    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
   LGR2A   8    23     15   32     3    11    32   36   16      LGR2 /
ENDFIN    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
         The LGRs of cartesian grid type are specified by the keyword CARFIN.
            The LGR is specified by the ijk-indexes. The data associated with
            this keyword are as follows:
            item 1 (name) - the name of LGR. Father, we can reference to the
               LGR by its name 'LGR1';
            items 2,3 (imin-imax) - the minimal and the maximal i-index of the
               parent grid, to which the LGR is applied;
            items 4,5 (jmin-jmax) - the minimal and the maximal j-index of the
               parent grid, to which the LGR is applied;
            items 6,7 (kmin-kmax) - the minimal and the maximal k-index of the
```

```
                parent grid, to which the LGR is applied;
             item 8 (ni) - the new number of cells along the i-indexation axis
                (ni>imax-imin);
             item 9 (nj) - the new number of cells along the j-indexation axis
                (nj>jmax-jmin);
             item 10 (nk) - the new number of cells along the k-indexation axis
                (nk>kmax-kmin);
             item 11 (parent_grid) - the name of the parent grid. By the
                default option, the parent grid is the whole reservoir.
          The grid LGR2A is nested in the grid LGR2.
          After the keyword CARFIN is executed, MUFITS automatically creates the
             the LGR and makes this grid active. The keyword ENDFIN makes the
             parent grid of the reservoir active. This keyword does not have
             associated data.

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

FAULTS
   ASCII '../NPD5_Faults.txt' /
          The faults are specified by the keyword FAULTS. This keyword has
             tabular associated data:
             item 1 - the fault ID (8 byte character); we can farther
                reference to the fault by this ID;
             items 2-7 - define cells, which have a face belonging
                to the fault. The cells are defined using the ijk-indexation
                box.
             items 8 - defines, which faces of the cells form the fault.
                This item must be any of X-,X+,Y-,Y+,Z-,Z+,I-,I+,J-,J+,K-,K+.
          The keyword FAULTS can be tuned up to load the fault specification
             from an include file. If the 1st argument of this keyword is the
             mnemonic ASCII then  the loading is invoked. In this case the 2nd
             argument is the system path to the include file. The mnemonic ASCII
             signifies that the include file is the formatted file.
          In the include file the following faults are defined: FAULT3, FAULT5,
             FAULT6, FAULT9, FAULT10.

MULTFLT
-- --name--  -multiplier-
   FAULT3     0.1 /
   FAULT5     0.1 /
   FAULT6     0.1 /
   FAULT9     0.1 /
   FAULT10    0.1 /
-- --------  ------------
/
          The transmissibility multiplier across the fault is specified by
             the keyword MULTFLT. This keyword has tabular associated data.
             item 1 - the fault ID defined by the keyword FAULTS;
```

```
            item 2 - the transmissibility multiplier.
         According to the computational problem formulation the transmissibility
            across every fault must be multiplied by 0.1.

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


BOUNDARY
-- --name--  ------box------  --direction tags--  --type--  --mode--
    123      6*                I- I+ J- J+ 2*     SAMESIZE /
-- --------  --------------  ------------------  --------  --------
/
         Before defining the boundary conditions in the section INIT, we must
            define the boundaries itself within these brackets MAKE/ENDMAKE.
            The boundaries are defined using the keyword BOUNDARY, which has
            tabular associated data: every row for a new boundary. The data
            items are as follows:
            item 1 - the boundary ID (an integer). The auxiliary cells,
               which MUFITS creates for the boundary are marked out by the
               condition FLUXNUM=ID.
            items 2-7 - define a region of the reservoir (i=[imin,imax],
               j=[jmin,jmax], k=[kmin,kmax]), for which the boundary is
               defined. By default, this region is the whole active grid (e.g.
               in the first data row i=[1,78], j=[1,78], k=[1,9]).
            items 8-13 - the direction tags (any of X-,X+,Y-,Y+,Z-,Z+,I-,I+,
               J-,J+,K-,K+). These tags define, which faces of the cells in
               the region form the boundary.
            item 14 - the type of the cells, which MUFITS creates for the
               boundary (8 byte character). The possible values are:
                  SAMESIZE - MUFITS creates the cells, which have the same
                     geometrical volume and distance to the interface as the
                     cell in the region defined by the items 2-7, to which
                     the created cell is connected (default value).
                  INFTHIN - MUFITS creates infinitely thin cells.
            item 15 - the creation mode (8 byte character). The possible
               values are:
                  ACTBASED - MUFITS creates the auxiliary cells for every
                     cell in the region defined by the items 2-7, which does
                     not have an active cell connected to its face defined
                     by the items 8-13 (default value).
                  ALL - MUFITS creates the auxiliary cells for every cell
                     in the region defined by the items 2-7 regardless the
                     distribution of the property ACTNUM.
         Using the keyword BOUNDARY we define the outer boundary of the
            reservoir. We use the default mode ACTBASED in order not to
            influence the internal regions of the reservoir.

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

```

```
SRCSPECG
-- ---ID---  --i--  --j--  --k--  -xcoord-  -ycoord-  --depth--
      106      58     48     6  /
      107      58     48     7  /   decomment this three
      110      58     48     10 /   lines for the scenario INJ1
-- --------  -----  -----  -----  --------  --------  ---------
--    106      64     47     6  /
--    107      64     47     7  /   decomment this three
--    110      64     47     10 /   lines for the scenario INJ2
-- --------  -----  -----  -----  --------  --------  ---------
/
          The point sources can be specified using the keyword SRCSPECG
             within the brackets MAKE/ENDMAKE. The tabular data associated
             with this keyword are as follows:
             item 1 - the source ID (4 byte integer);
             item 2 - the i-index of the cell in the active grid, to which the
                source is connected;
             item 3 - the j-index of the cell in the active grid, to which the
                source is connected;
             item 4 - the k-index of the cell in the active grid, to which the
                source is connected;
             item 5 - the x-coordinate of the point source;
             item 6 - the y-coordinate of the point source;
             item 7 - the z-coordinate (depth) of the point source.
          We can speicfy either the ijk-indexes of the cell, to which the
             the source is connected or its spatial coordinates. On the first
             hand MUFITS tries to use the ijk-indexes.

          According to the scenario INJ1 the injection well is
             perforated in cells (i=58, j=48, k=6), (i=58, j=48, k=7) and
             (i=58, j=48, k=10). In the current study we replace every
             perforation of the well by a point source. We have 3 sources which
             are specified by the keyword SRCSPECG.

          If you want to simulate the scenario INJ1 then decoment only the first
             three data lines associated with the keyword SRCSPECG.
          If you want to simulate the scenario INJ2 then decoment only the last
             three data lines associated with the keyword SRCSPECG.

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

SAVEMVS
/
          The keyword SAVEMVS targets MUFITS to save the MVS-file for the
             grid defined within the current MAKE/ENDMAKE brackets. This keyword
             has the name of the file as the associated data. We use the default
             name of the file 'EXAMPLE-H4.MVS'.

```

```
ENDMAKE   >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>

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

LOADING   ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
   IJK /
          The keyword LOADING affects the following keywords PORO, PERMI.
             This keyword has one associated data item. The mnemonic IJK
             targets MUFITS to load data from files according to ijk-indexation
             in the current input box. MUFITS assumes that every loaded file
             contains the values of the properties (PORO, PERMI)
             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.

PORO
   ASCII '../NPD5_Porosity.txt' /
          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 NPD5_Porosity.txt 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 '../NPD5_Permeability.txt' /
          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).

COPY
-- --from-- ---to--- ------box------
   PERMI    PERMJ    /
   PERMI    PERMK    /
-- -------- -------- ---------------
/

MULTIPLY
-- --property-- --multiplier-- ------box------
      PERMK           0.1      /
```

```
-- ------------ -------------- ---------------
/
          According to the computational problem formulation, the following
             relations are hold:

                    PERMJ=PERMI
                    PERMK=0.1*PERMI   (the permeability ratio is 10)

          This specification can be done by copying the property PERMI to
             the properties PERMJ and PERMK. This operation can be done by the
             keyword COPY. This keyword has the following tabular associated
             data:
             item 1 - the mnemonic of the property, from which values are
                copied;
             item 2 - the mnemonic of the property, to which values are
                copied;
             item 3-8 - the input box in the active grid. The operation is
                applied only to the cells belonging to the box.
          Farther, we multiply the property PERMK by 0.1. This operation can be
             done by the keyword MULTIPLY. This keyword has the following
             tabular associated data:
             item 1 - the mnemonic of the modified property;
             item 2 - the multiplier value;
             item 3-8 - the input box in the active grid. The operation is
                applied only to the cells belonging to the box.

          Note that we don't define the petrophysical properties in the
             auxiliary cells, which MUFITS creates for the boundaries. If the
             petrophysical properties in these cells are not defined after the
             section REGIONS then MUFITS copies these properties from the
             cells, to which the auxiliary cells are connected.

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

REGALL    ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
          The switch REGALL does not have associated data. This keyword targets
             MUFITS to perform operations on array for all cells in the
             simulation but not only for the cells in the current input box.
             This keyword affects the data processing by the following keyword
             EQUALREG, which is related to the auxiliary cells of the boundary
             condition. It also affects the boundary conditions specification
             in the section INIT.

EQUALREG
--          new
-- property value    marker    marker value
-- -------- -------- --------- ---------
   FIPNUM   1        FLUXNUM   123       /
```

```
-- -------- -------- --------- ---------
/
          The fluid-in-place regions are defined by the property FIPNUM. By
             default, FIPNUM=0 in every cell. If we want to calculate the fluxes
             between the reservoir and its boundaries then we have to redefine
             the property FIPNUM in all auxiliary cells. We use the keyword
             EQUALREG to set FIPNUM=11 in all auxiliary cells. Thus, the
             reservoir itself is marked out as FIPNUM=0 while its boundaries
             are marked out as FIPNUM=1.

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

RPTRES
   MPINUM DEPTH PORO PERMI PERMJ PERMK MPINUM XCOORD YCOORD
                                  I_IJKRES J_IJKRES K_IJKRES /
          We specify the properties we want to save in the file
             'EXAMPLE-H4.GRID.SUM' after the section REGIONS. The file will
             contain the properties MPINUM, DEPTH, PERMI, etc.

SAVERES
   /
          Using the keyword SAVERES we target MUFITS to save
             'EXAMPLE-H4.GRID.SUM' file after the section REGIONS.
             We do not want to change the name of the summary file. That's why
             we do not modify the default data item 'EXAMPLE-H4.GRID.SUM'
             of the keyword SAVERES.

                              The section PROPS begins
PROPS     ##########################################################################
          In this section, we must define the thermophysical properties of
             binary mixture, host rock as well as the relative permeability
             curves.

LOADEOS
   '../../INCLUDE/CO2H2O_V3.0.EOS' /
          The keyword LOADEOS is used for loading the mixture properties from
             the EOS-file. This keyword has as associated data the system path
             to the file.

          The rock properties for every region ROCKNUM are specified within
             the brackets ROCK/ENDROCK.
ROCK      <<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<
   0 /
          The opening bracket ROCK has one associated data item, which is the
             ROCKNUM region ID. By default, all cells belong to the region
             ROCKNUM=0. Therefore, we set the data item to 0.

RMODEL1
```

```
-- grain density                heat capacity
--  [kg/m^3]                     [kJ/kg/K]
      2500.          4*             1.0 /
          The easiest way for the rock properties specification is by using the
             keyword RMODEL1.
          The first data item associated with this keyword is the host rock
             density.
          The record 4* means that we leave the default values for the data
             items 2-5.
          The 6th data item associated with the keyword is the host rock heat
             capacity.

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
   0.100   0.0000  0.4284 /
   0.150   0.0020  0.3800 /
   0.204   0.0084  0.3292 /
   0.258   0.0281  0.2820 /      sH2O   - H2O-rich phase saturation
   0.313   0.0592  0.2382 /      krH2O  - H2O-rich phase relative permeability
   0.367   0.1017  0.1978 /      krCO2  - CO2-rich phase relative permeability
   0.421   0.1555  0.1610 /
   0.475   0.2206  0.1276 /
   0.529   0.2971  0.0976 /
   0.583   0.3850  0.0712 /
   0.638   0.4842  0.0482 /
   0.692   0.5948  0.0286 /
   0.746   0.7167  0.0126 /
   0.800   0.8500  0.0000 /
/
          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.
          The relative permeabilities represent an assembly of the data from
             the files Scaled_RelPermWater.txt and Scaled_RelPermCO2.txt.
```

```

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

PHASES
-- name   pres  enth  CO2 H2O  crit._saturation
   LH2O   1.0    5.0  0.0 1.0      0.1         /
   SCO2   10.0  10.0  1.0 0.0      0.2         /
/
          The keyword PHASES defines new MNEMONICS for data output. This keyword
             defines tabular data and every row of these data defines an
             individual phase. The 1st column is the phase name (no more
             than 4 characters). The following data items defines typical
             thermodynamic parameters of the phase. The 2nd column is the
             pressure, the 3rd is the enthalpy, the 4th and 5th are the molar
             composition of binary mixture. The 6th column is the critical
             saturation of the phase, which affects the properties MM1#NAME,
             MM2#NAME, MC1#NAME, MC2#NAME. By default, this critical saturation
             is equal to 0.
          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
-- -------- -------- --------- --------- -------- -------- -------- ---------
   PRES     DEPTH    SATNUM    0         MULTA    0.31     0.01              /
   TEMP     DEPTH    SATNUM    0         MULTA    283      0.03              /
-- -------- -------- --------- --------- -------- -------- -------- ---------
/
          We use the keyword OPERAREG to specify the initial distribution of
             pressure and temperature. 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'.

          The first data row associated with the keyword OPERAREG defines the
             following hydrostatic distribution of the pressure:

                PRES=0.31+0.01*DEPTH.

          Here, we suppose that the water density is 1000 kg/m^3, and that
             the pressure at the reference depth 3100 meters is 31.31 MPa.
          The second data row associated with the keyword OPERAREG defines the
             following distribution of the temperature:

                TEMP=283+0.03*DEPTH.

          Here, we suppose that the geothermal gradient is 3 degrees per 100
             meters, and that the temperature is 100 C at the reference depth
             3000 meters.

EQUALREG
--           new
-- property value    marker    marker value
-- -------- -------- --------- ---------
   COMP1T   0.0      SATNUM    0         /
-- -------- -------- --------- ---------
/
          Using the keyword EQUALREG we specify that the initial CO2 content
             is equal to 0. Thus, the reservoir is saturated by pure water.

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

RPTSOL
  PRESSURE TEMP ENTHT COMP1T COMP2T
    I_IJKRES J_IJKRES K_IJKRES
        SAT#LH2O  SAT#SCO2
        CP1#LH2O  CP1#SCO2
        CP2#LH2O  CP2#SCO2
        REL#LH2O  REL#SCO2
        MS1#LH2O  MS1#SCO2
        MC1#SCO2  MM1#SCO2 /
          The properties we want to save in the summary files during the
             simulation can be specified using 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 the 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.

RPTSRC
   FLUX1 FLUX2 FLUXE /
           The output for the point sources is specified by the keyword RPTSRC.
              MUFITS will save in the summary files:
                 FLUX1 - the current injection rate of the 1st component
                    for every source;
                 FLUX2 - the current injection rate of the 2nd component
                    for every source.

RPTFIP
   PRESSURE MASS1 MASS2 FLUX1 FLUX2 FLUXE MS1#LH2O MS1#SCO2 MC1#SCO2 MM1#SCO2 /
           The output for the fluid-in-place regions is initiated by the keyword
              RPTFIP. MUFITS will save in the summary files:
                 PRESSURE - the average pressure in every region FIPNUM;
                 FLUX1    - the current flux of the 1st component between the
                            regions FIPNUM;
                 FLUX2    - the current flux of the 2nd component between the
                            regions FIPNUM;
                 FLUXE    - the current energy flux between the
                            regions FIPNUM;
                 MS1#LH2O - the total mass of CO2 in water phase in every region
                            FIPNUM;
                 MS1#LCO2 - the total mass of CO2 in CO2-RICH PHASE in every
                            region FIPNUM
                 etc. (see the document "List of Mnemonics").

                            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*      1.8         5*      200                200  /
           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).

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

          The schedule description:

              name        duration                  description
             ------------------------------------------------------------
             Period1  -   1    year     -   hydrostatic conditions evaluation;
             Period2  -   100  years    -   the period of injection;
             Period3  -   2500 years    -   the post-injection period.

          The injection volume is 400 Mt of CO2 in 100 years.
          The injection rate = 10951.4031 t/day=3*3650.4677 t/day; Therefore the
             injection rate for every source is 3650.4677 t/day.

          The injection temperature = 80C = 353K if the pressure is equal to
             25 MPa

                                  The Period1 begins
          ========================================================================

OPTIONS
   20* 0 /
          The keyword OPTIONS is used to enable/disable simulation options.
             All data items associated with this keyword are either 1 (enabled)
             or 0 (disabled).
          The 21st argument of the keyword OPTIONS controls the application of
             the cascade method (potential ordering technique). If the flow is
             single-phase then it is better to disable the method, which will
             slow down the calculation.

TUNING
-- timestep setup
-- limit   max    next   min
    5      1000    365 /
          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
   365.25 /
          We proceed the simulation over 1 year (365.25 days) in the
             simulation schedule in order to evaluate good hydrostatics.

                                The Period2 begins
          ============================================================================

OPTIONS
   20* 1 /
          The cascade method is enabled.

EQUALREG
--          new
-- property value    marker    marker value
-- -------- -------- --------- ---------
   ACTNUM   2        FLUXNUM   123       /
-- -------- -------- --------- ---------
/
          After the hydrostatics is evaluated, we can fix parameters at the
             boundaries. This is done by using the keyword EQUALREG. The
             property ACTNUM is set to 2 in all cells marked out as
             FLUXNUM=123.

SRCINJE
--  ID    mode    target    Mrate     pres     enth    co2   h2o    temp
--                          [t/day]   [MPa]  [kJ/mol]                [K]
   106    OPEN     FINJ    3650.4677   25.       1*    1.0   0.0    353  /
   107    OPEN     FINJ    3650.4677   25.       1*    1.0   0.0    353  /
   110    OPEN     FINJ    3650.4677   25.       1*    1.0   0.0    353  /
/
           The parameters of the injection are specified by the keyword
              SRCINJE, which has tabular associated data. In every line of the
              table the 1st data item is the source ID (see the keyword
              SRCSPECG in the section GRID).
           The 2nd data item is the source mode, which is OPEN - the
              injection occurs (if the mode is SHUT then the injection does
              not occur).
           The 3rd data item is the injection target FINJ, which specifies
              that the injection occurs under fixed injection rate condition.
           The 4th data item is the injection rate (3650.4677 t/day).
           The 5th data item is the reference pressure (25 MPa)
           The 6th data item is not used in this example.
           The 7th and 8th data items are the injected mixture composition
```

```
              (1.0,0.0). Pure CO2 is injected using the point sources.
           The 9th data item is the temperature of the mixture (353 K) under
              the reference conditions (if the pressure = 25 MPa).

TUNING
-- timestep setup
-- limit   max    next   min
    1.     365.5   10. /

TSTEP
   50*730.5 /
          We proceed the simulation over 100 years (50*730.5 days) in the
             simulation schedule. The output is saved after every 2 years in
             the schedule.

                                  The Period3 begins
          ============================================================================

SRCOPEN
--  ID     mode
-- ------- --------
   106     SHUT     /
   107     SHUT     /
   110     SHUT     /
-- ------- --------
/
          As the Period3 is the post-injection period we must stop the CO2
             injection through the point sources. This can be done by changing
             the mode of every source from OPEN to SHUT. The easiest way to do
             this is by the keyword SRCOPEN, which has the following associated
             data:
             item 1 - the source ID;
             item 2 - the source mode.
          The injection is stopped after this keyword is executed.

TUNING
-- timestep setup
-- limit   max    next   min
    1.     1840    10. /

TSTEP
   50*3652.5 /
          We proceed the simulation over 500 years (50*3652.5 days) in the
             simulation schedule. The output is saved after every 10 years in
             the schedule.

TUNING
-- timestep setup
```

```
773 -- limit   max    next   min
774     1*    3653    1* /
775
776 TSTEP
777    100*7305.00 /
778           We proceed the simulation over 2000 years (100*7305.00 days) in the
779              simulation schedule. The output is saved after every 20 years in
780              the schedule.
781
782                 The section SCHEDULE must be terminated by the keyword END
783 END         ########################################################################
784
785 MUFITS does not read the following records.
```

1.4. 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-H4 in the folder SIMULATIONS. Navigate to the folder EXAMPLE-H4;

7. copy the files NPD5.grdecl, NPD5_Porosity.txt, NPD5_Permeability.txt, NPD5_Faults.txt to the folder EXAMPLE-H4;
8. create the folder RUN1 in the folder EXAMPLE-H4;
9. copy the file EXAMPLE-H4.RUN to the folder RUN1;
10. navigate to the folder RUN1;
11. create the text file EXAMPLE-H4.BAT in the folder RUN1;
12. type the following command in the file EXAMPLE-H4.BAT: "C:/Program Files (x86)/MPICH2/bin/mpiexec.exe" -n 8 ../../BIN/H32.EXE EXAMPLE-H4.RUN > EXAMPLE-H4.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 8' defines that 8 processes are 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-H4.BAT;
13. execute the file EXAMPLE-H4.BAT (double click on this file).

1.5. Output data

The following files are created by MUFITS in the directory SIMULATIONS/EXAMPLE-H4/RUN1/ after the successful simulation:

Output files		
EXAMPLE-H4.LOG	-	the simulation LOG-file;
EXAMPLE-H4.MVS	-	the MVS-file for the considered problem;
EXAMPLE-H4.GRID.SUM	-	the SUM-file saved after the section REGIONS;

EXAMPLE-H4.0000.SUM, EXAMPLE-H4.0001.SUM,..., EXAMPLE-H4.0201.SUM	-	the SUM-files for different times in the simulation schedule.

1.6. Simulation results

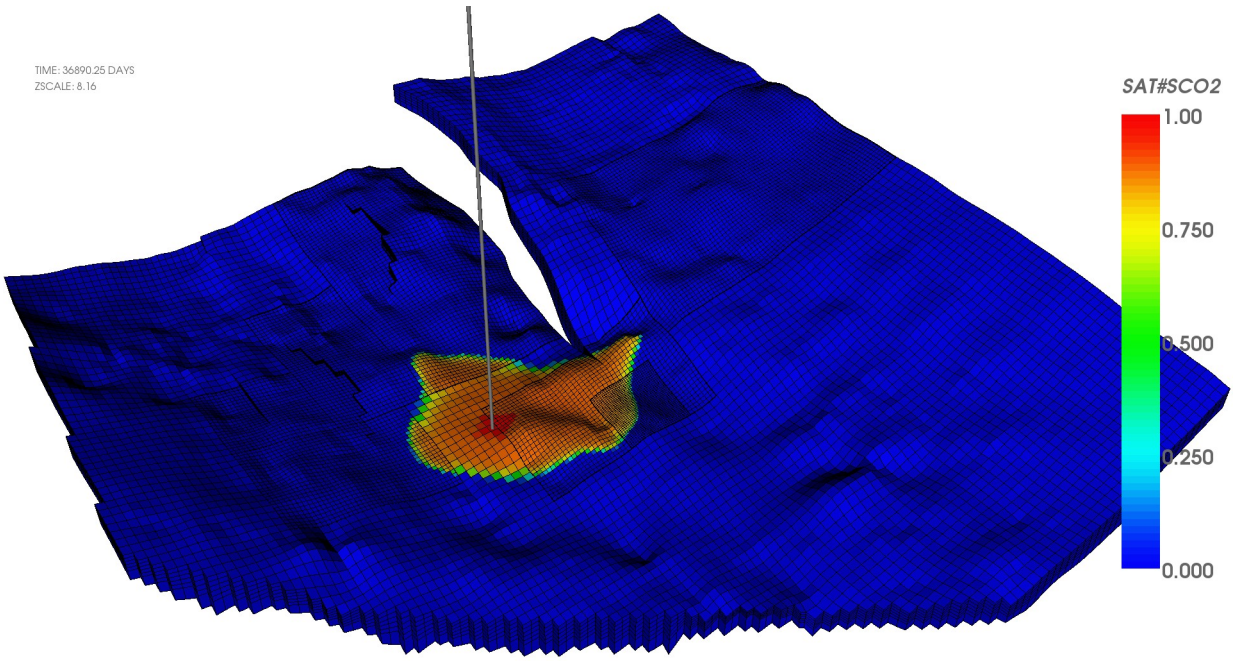

Figure 1.2: CO_2 saturation in the top layer of the Jonansen formation for the scenarion INJ1. t=100 years.

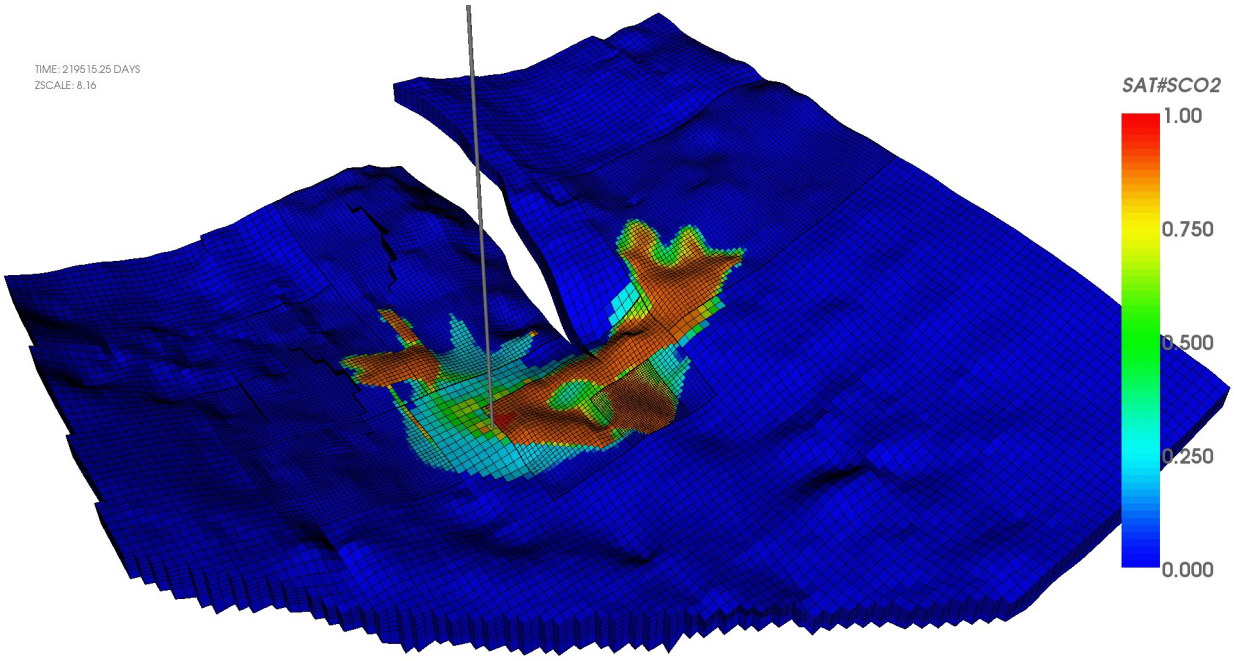

Figure 1.3: CO_2 saturation in the top layer of the Jonansen formation for the scenarion INJ1. t=600 years.

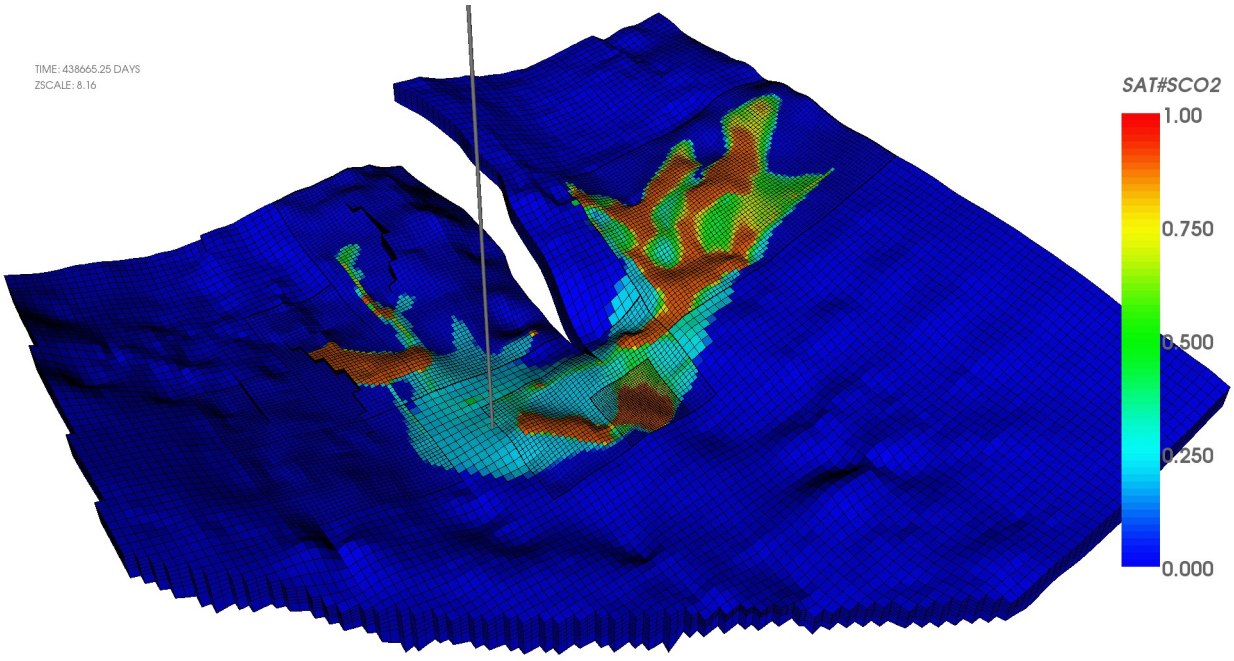

Figure 1.4: CO_2 saturation in the top layer of the Jonansen formation for the scenarion INJ1. t=1200 years.

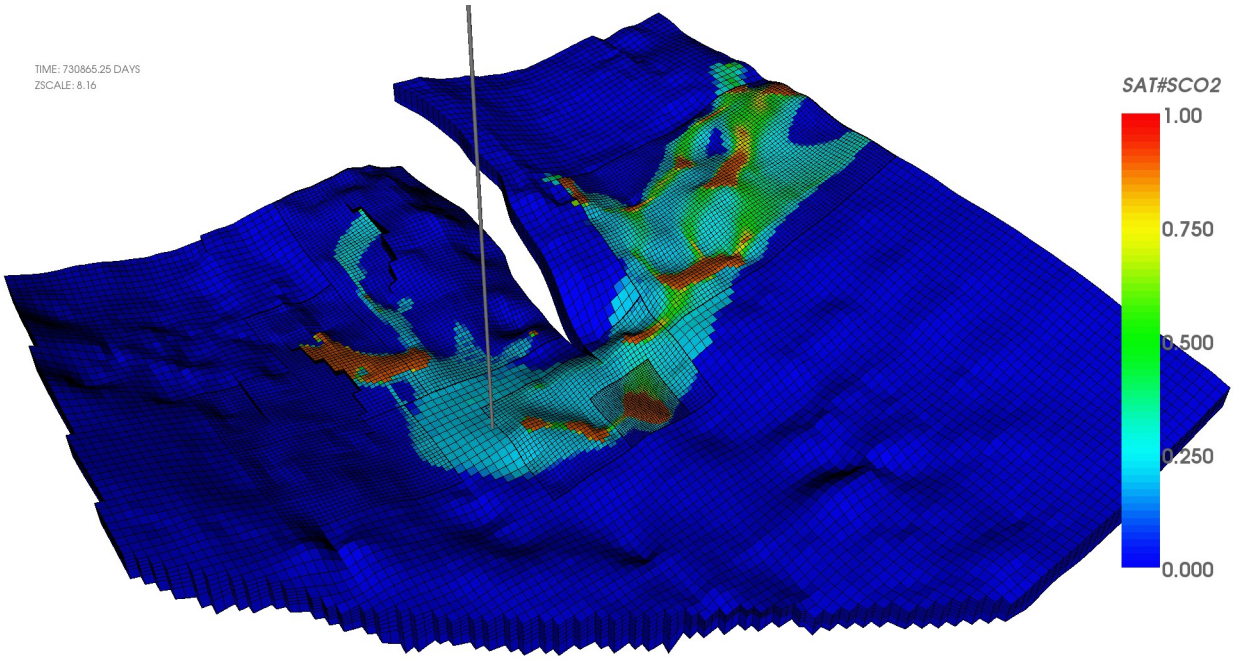

Figure 1.5: CO_2 saturation in the top layer of the Jonansen formation for the scenarion INJ1. t=2000 years.

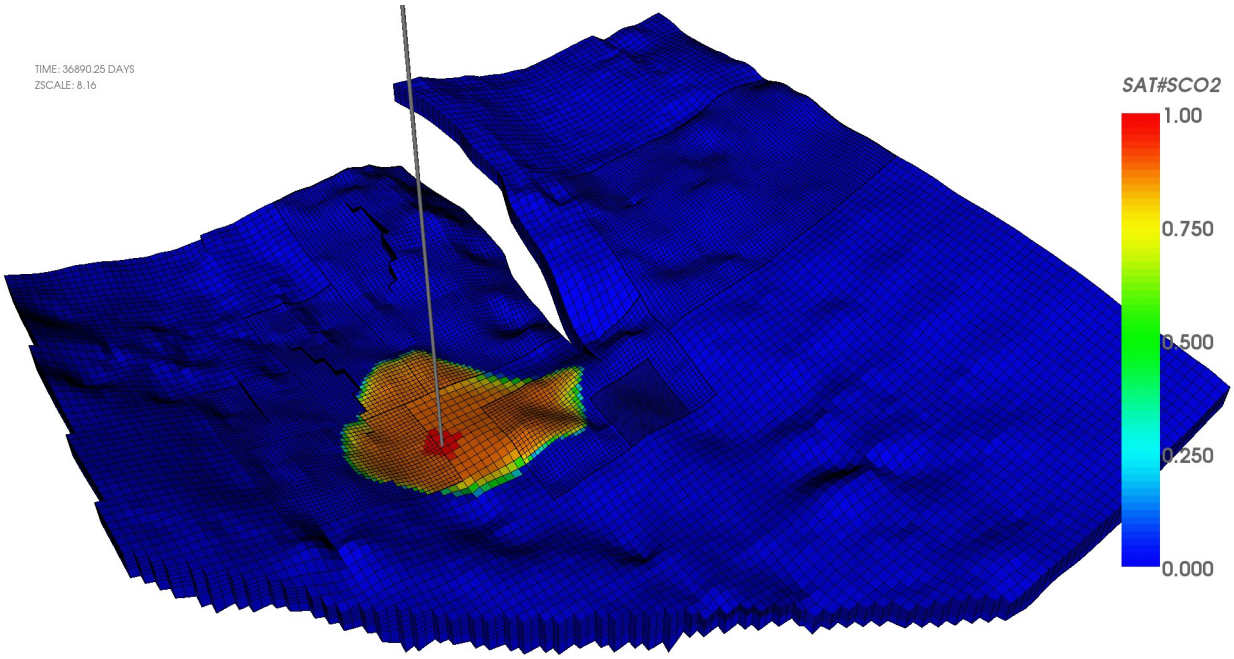

Figure 1.6: CO_2 saturation in the top layer of the Jonansen formation for the scenarion INJ2. t=100 years.

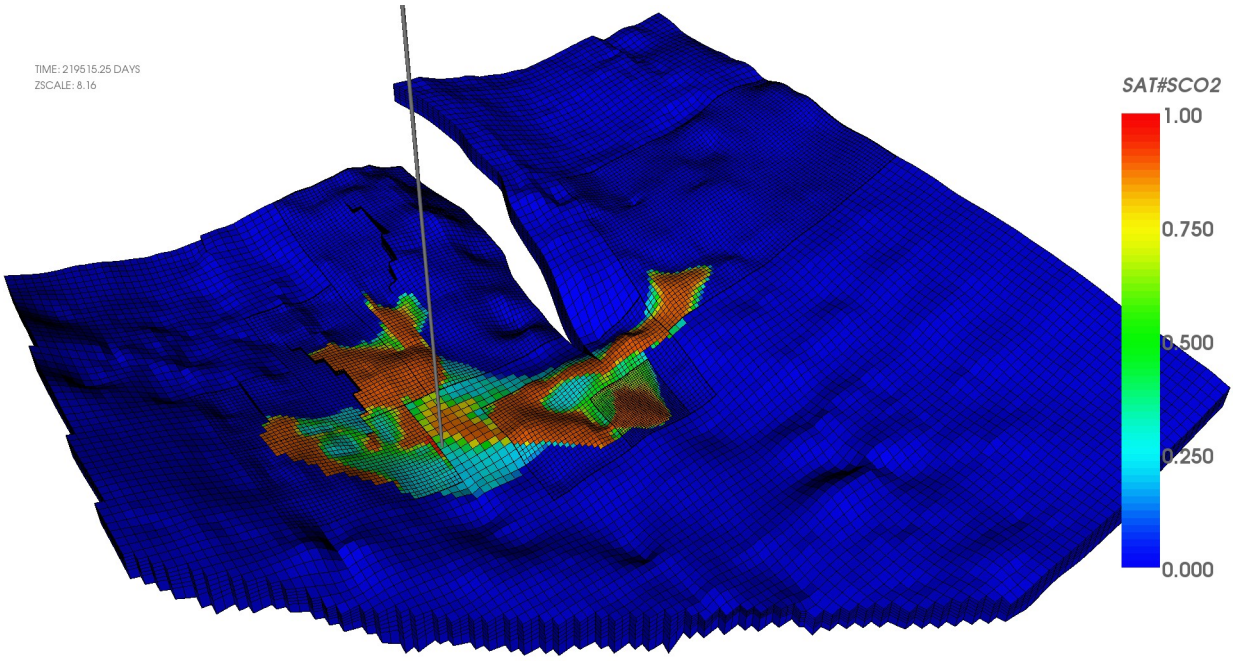

Figure 1.7: CO_2 saturation in the top layer of the Jonansen formation for the scenarion INJ2. t=600 years.

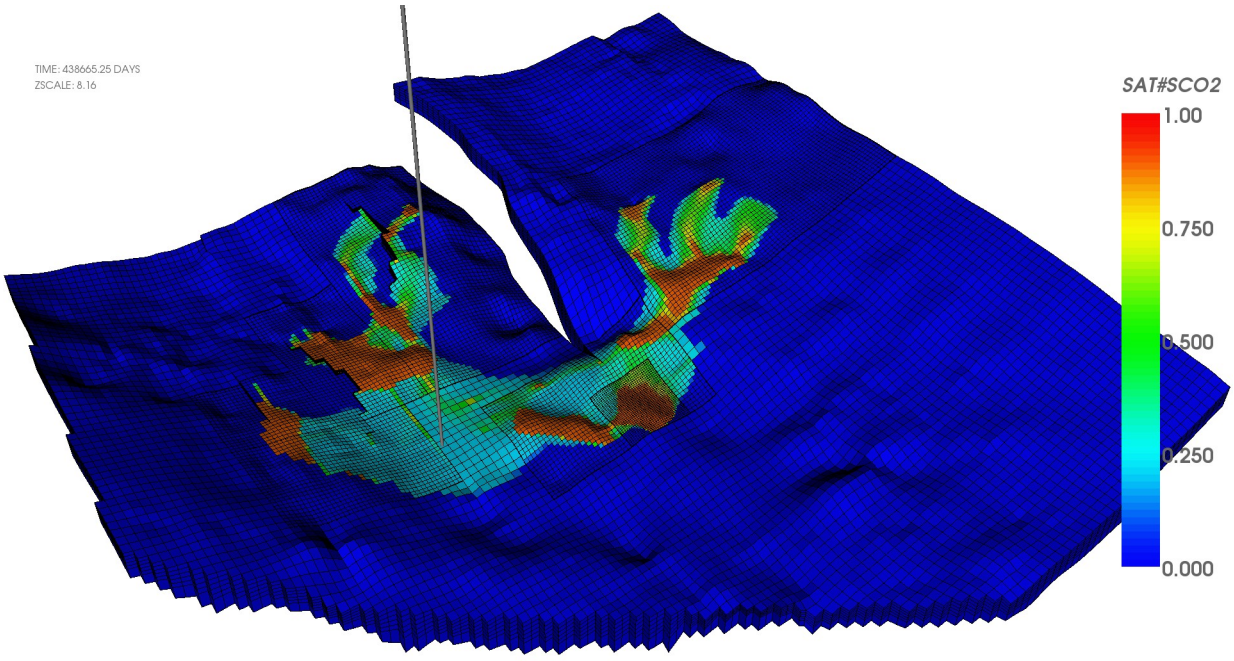

Figure 1.8: CO_2 saturation in the top layer of the Jonansen formation for the scenarion INJ2. t=1200 years.

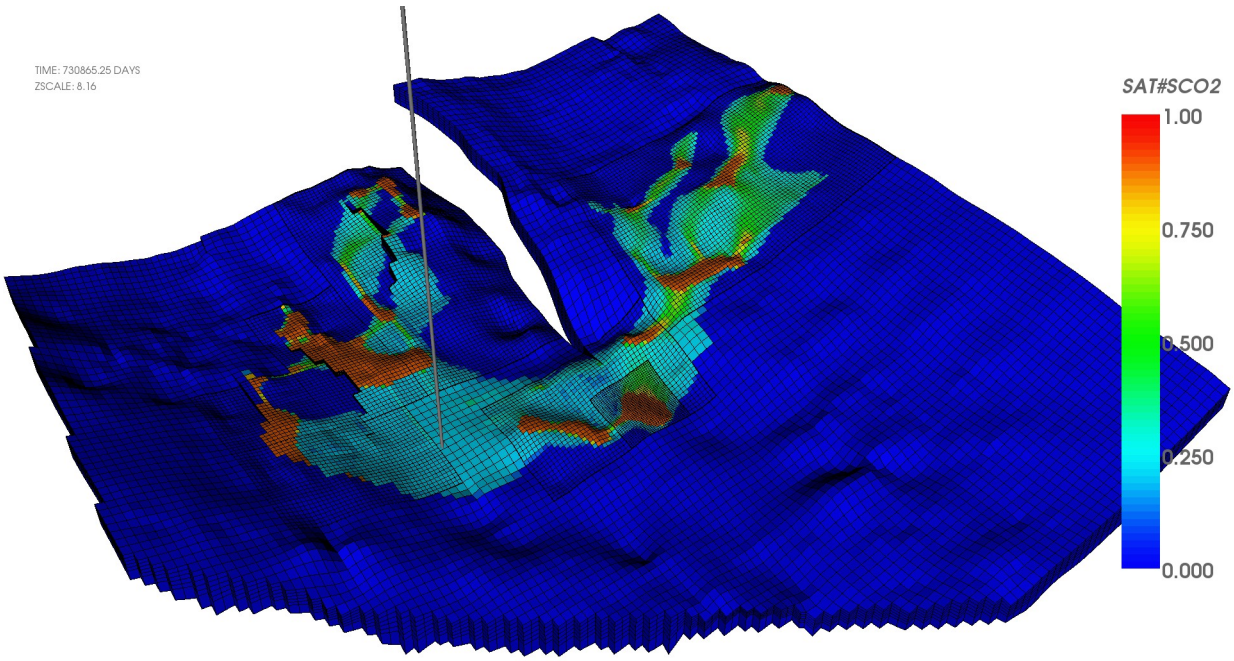

Figure 1.9: CO_2 saturation in the top layer of the Jonansen formation for the scenarion INJ2. t=2000 years.

References

1. www.sintef.no/Projectweb/MatMorA/Downloads/Johansen/

2. *Eigestad GT, Dahle HK, Hellevang B, Johansen WT, Riis F, Oian E.* Geologic modeling and simulation of CO_2 injection in the Johansen formation. Comput Geosci 2009; 13: 435-50.

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