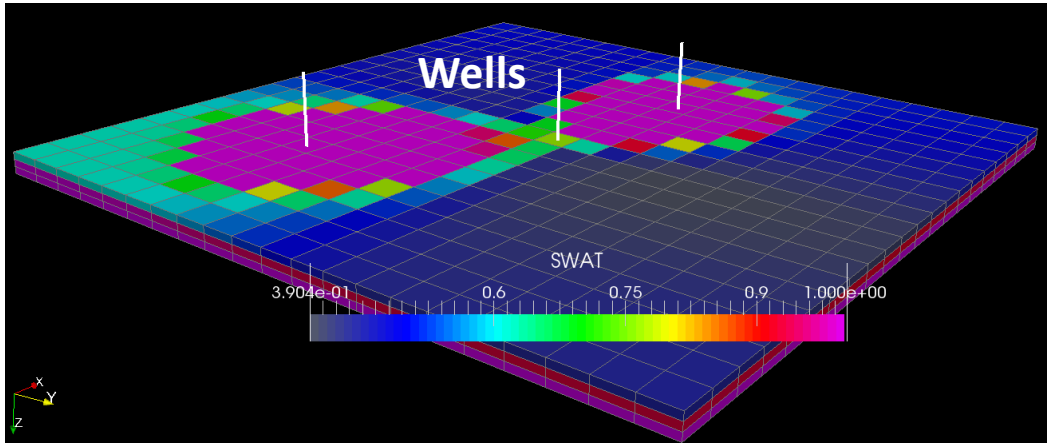
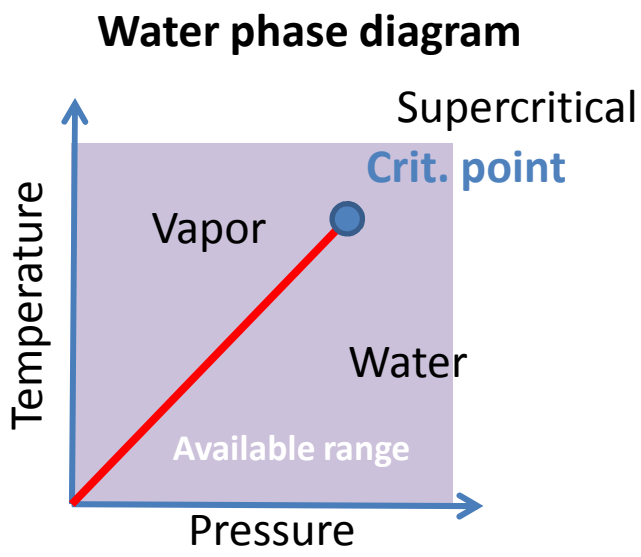
MUFITS
Training Course

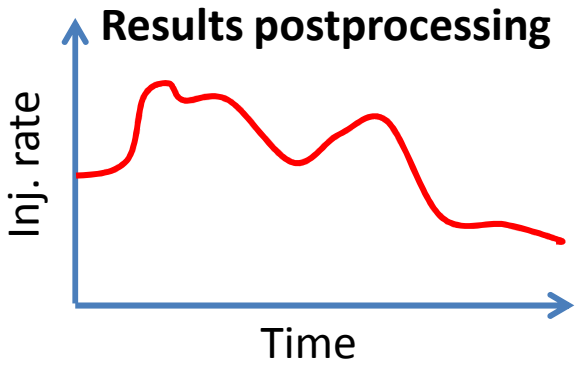
Day 3
Module BINMIXT, Section POST
& Wells

Program

- BINMIXT EOS module (scenario 5)
- Section POST
- Wells (scenario 6)







BINMIXT EOS module

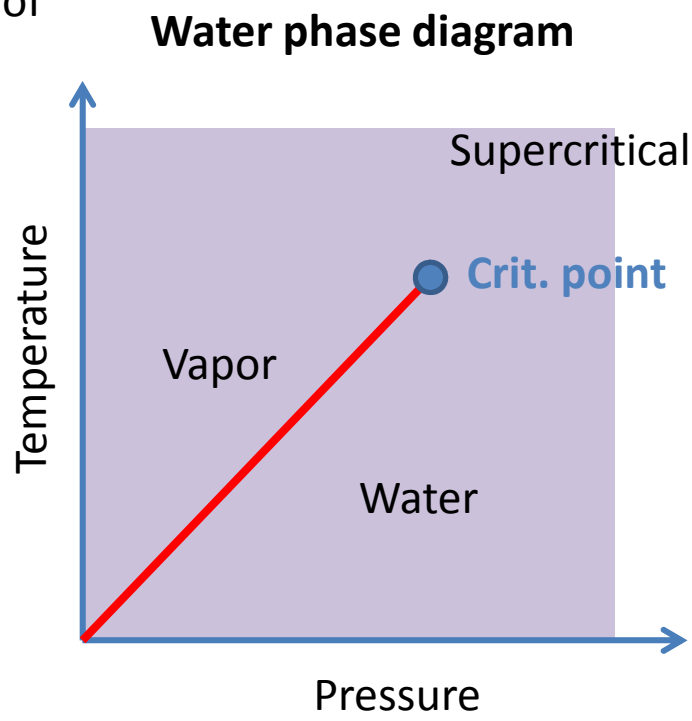
EOS module description

BINMIXT module is designed for nonisothermal modelling of multiphase flows of binary mixture in a wide range of pressures and temperatures and under near critical thermodynamic conditions.

The module is capable of modelling three-phase flows of binary mixture.

BINMIXT is the default module of the simulator.

This courses covers application of the module for CO_2-H_2O flows. The available range of pressures is <0.01 bars to >1500 bars. The available range of temperatures is 0 °C to >900 °C.



Primary variables

For robust hydrodynamic simulations in the vicinity of critical conditions, a non-classic variables must be used: pressure-enthalpy-composition.

classic approach

P, T, x

pressure, temperature, composition

"Flash" calculation (evaluation of thermodynamic equilibrium). Cubic equation of state is used

Only 1- and 2-phase states of the mixture:

liquid (H_2O) | **gas** ($sc.CO_2$)

possible phases

the proposed approach

P, h, x

pressure, enthalpy, composition

A generalization of classic "flash" calculation

1-, 2- and **3-phase** states of the mixture:

liquid (H_2O) | **liquid** ($l.CO_2$) | **gas** ($g.CO_2$)

possible phases

Mathematical model

Balance equation

$$\frac{\partial}{\partial t}\left(m\sum_{i=1}^{3}\frac{M_{(j)}x_{i(j)}}{v_i}s_i \right)+$$

- mass conserv.

$$+\operatorname{div}\left(\sum_{i=1}^{3}\frac{M_{(j)}x_{i(j)}}{v_i}\mathbf{w}_i \right)=0,\quad j=1,2$$

$$\frac{\partial}{\partial t}\left(m\sum_{i=1}^{3}\frac{e_i}{v_i}s_i+(1-m)\frac{e_s}{v_s} \right)+$$

- energy conserv.

$$+\operatorname{div}\left(\sum_{i=1}^{3}\frac{h_i}{v_i}\mathbf{w}_i-\lambda\mathbf{grad}T \right)=0$$

$$\mathbf{w}_i=-K\frac{f_i}{\mu_i}\left(\mathbf{grad}P-\frac{M_i}{v_i}\mathbf{g} \right)$$

- Darcy correlation

Equations are in molar variables

+

Equations for prediction

$$\sigma_t=\sum_{i=1}^{3}\sigma_i V_i\to\max,$$

$$\sigma_i=\sigma\left(P,h_i,x_i\right),\qquad \sum_{i=1}^{3}V_i=1$$

$$\sum_{i=1}^{3}h_i V_i=h_t,\qquad \sum_{i=1}^{3}x_i V_i=x_t$$

$$0\le V_i\le 1$$

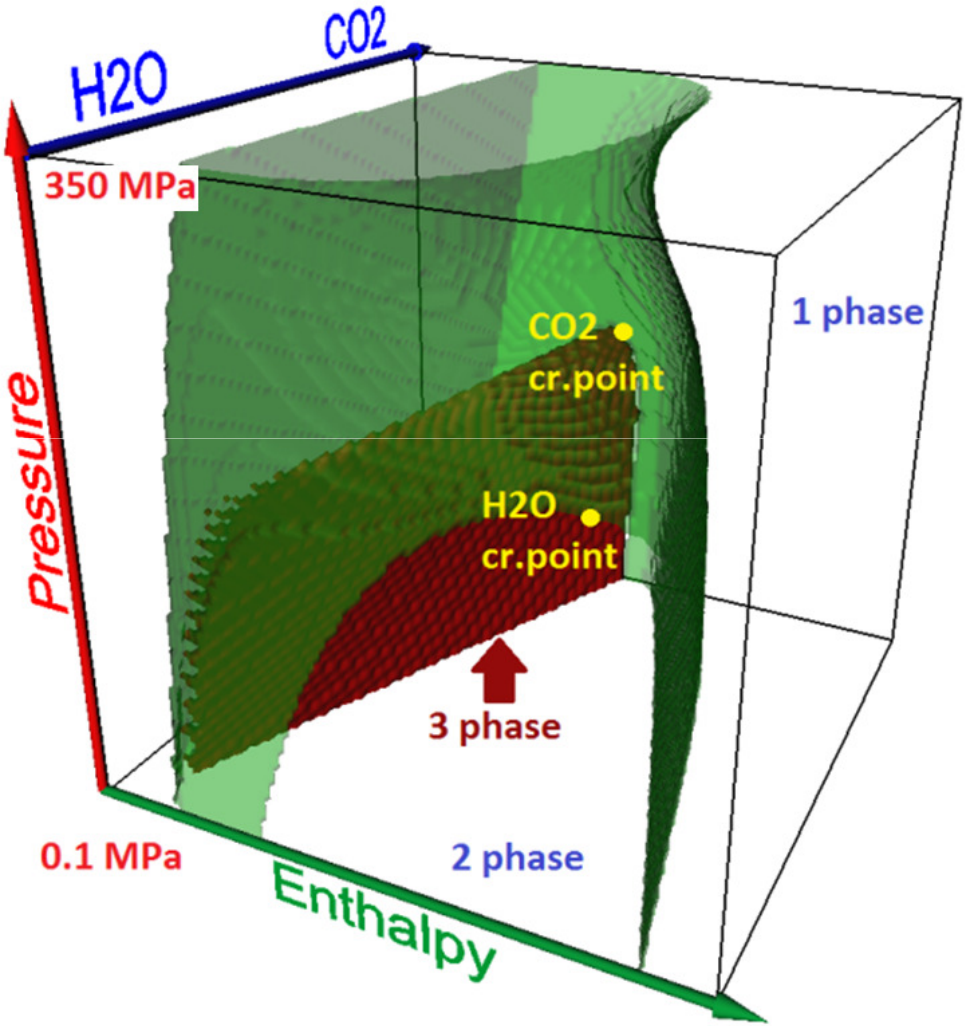
$j=1$ – CO_2

$j=2$ – H_2O

P – pressure, h – enthalpy

x – composition, σ – entropy

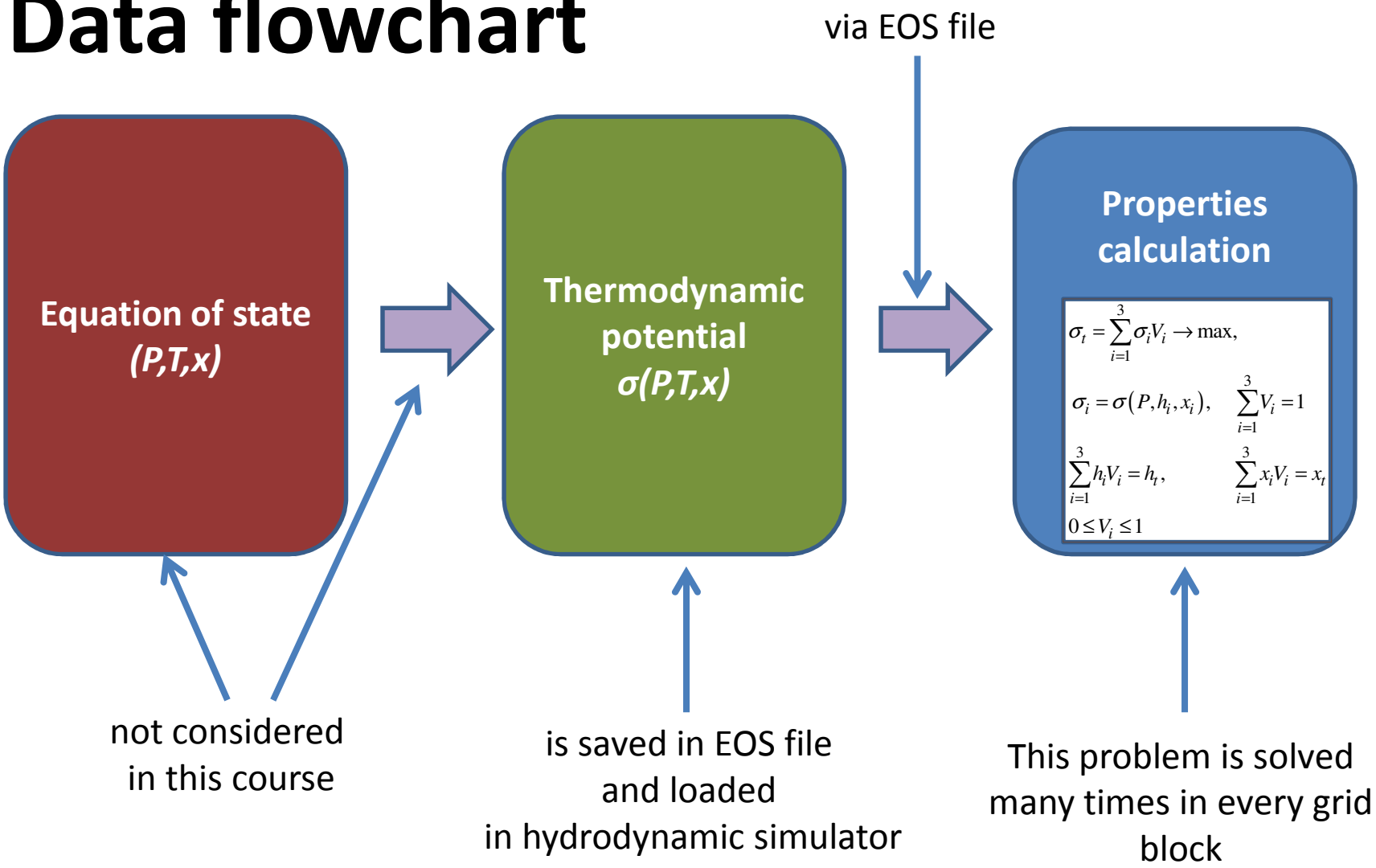
CO_2-H_2O phase diagram



Phase diagram in pressure-enthalpy-composition variables

Outside green surface - single-phase states, inside green and outside red surface – two-phase states, inside red surface – three-phase states.

Data flowchart



LOADEOS keyword

The EOS-file contains the thermodynamic potential of the mixture which was calculated in advance. The file should be copied in INCLUDE folder. The file must be loaded by the **LOADEOS** keyword in **PROPS** section.

LOADEOS syntax

```
-- in PROPS section

LOADEOS
   filename /

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

   filename - name of EOS file.
```

Additional mnemonics

Mnemonic	Description
ENTHT	Total molar enthalpy (kJ/mol)
COMP1T	Total molar fraction of the 1st component (CO_2)
COMP2T	Total molar fraction of the 2nd component (H_2O)
SGASINIT	Initial gas saturation
SLIQINIT	Initial liquid saturation

Initial conditions

Initial conditions options:

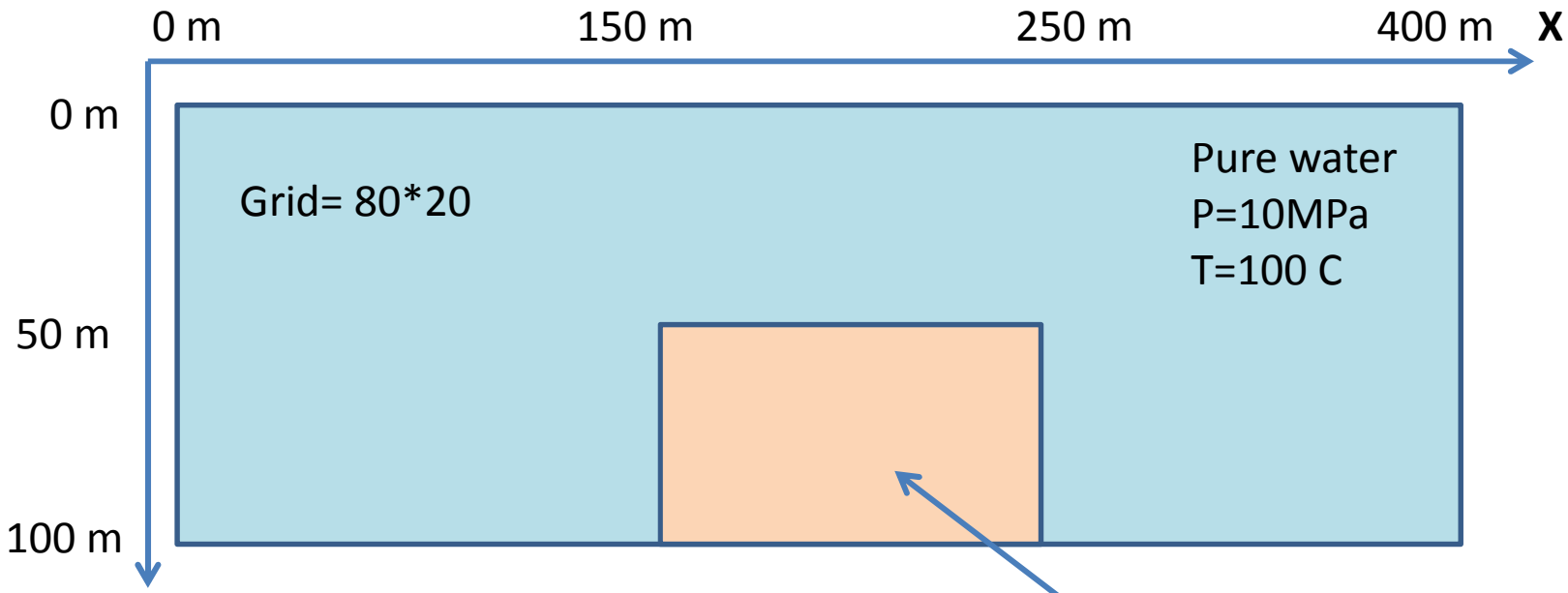
a) Pressure (PRES), Temperature (TEMP or TEMPC), Composition (COMP1T or COMP2T) [priority 1];
b) Pressure (PRES), Enthalpy (ENTHT), Composition (COMP1T or COMP2T) [priority 2].

For two-phase states defined by a) and b) the saturations of phases can be redefined by the SLIQINIT and SGASINIT mnemonics. Note, that in this case, the total enthalpy (ENTHT) and total compositions (COMP1T or COMP2T) are altered to satisfy the conditions for saturation, however the thermophysical properties of each phase (density, viscosity, etc.) are not altered.

Scenario 5

Simulate scenario up to 200 days reporting solution every 10 days.

Rock properties:
Porosity = 0.25;
Permeability = 100 mD ;
Rock density = 2900 kg/m^3;
Heat capacity = 1 kJ/kg/K;
Heat conduct. = 2 W/m/K.



Rel. Permeabilities
Brocks and Corey,
s_{min}=0.2, s_{max}=0.95

$$k_{r,l} = s_l^4$$

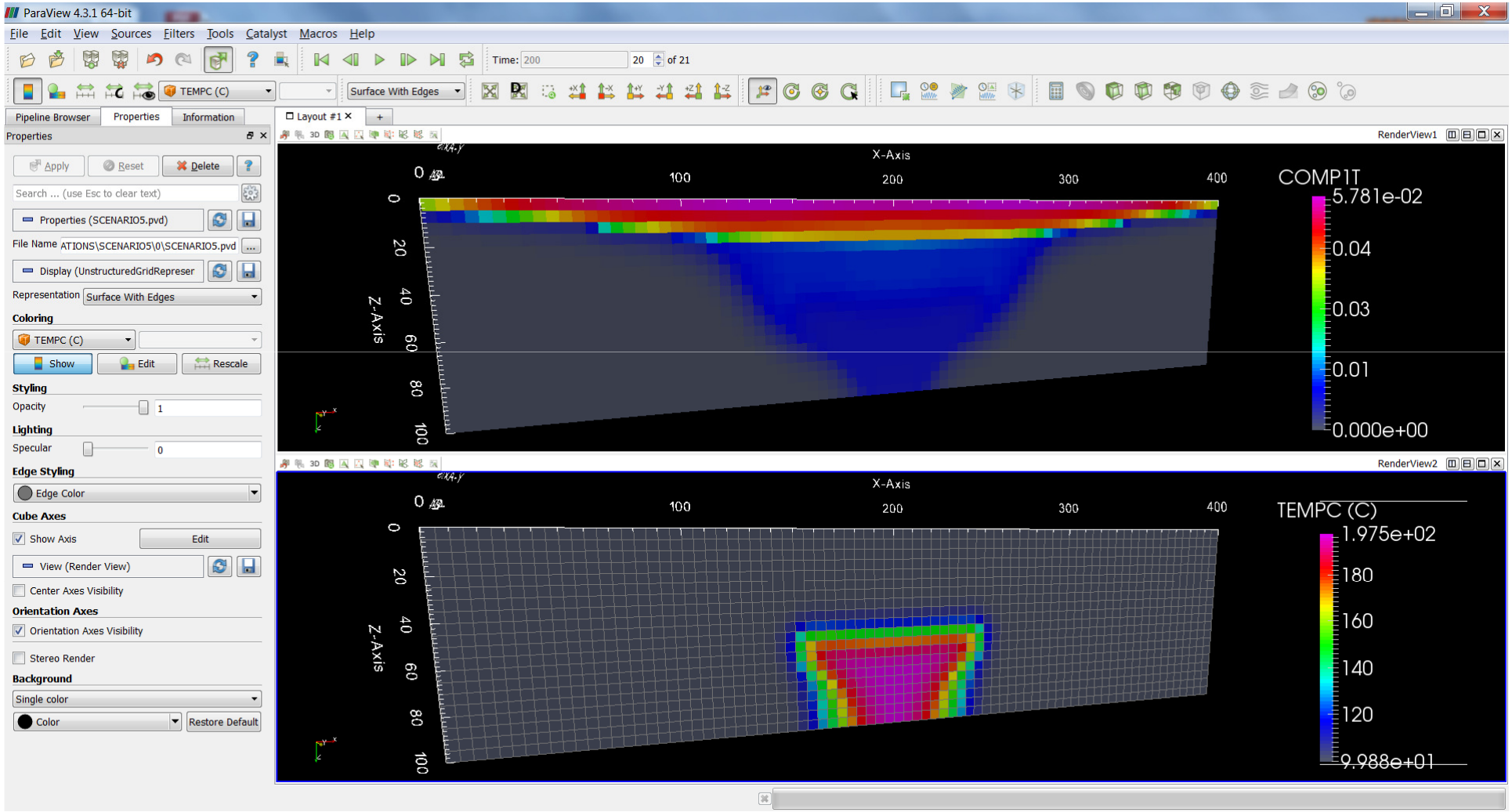
$$k_{r,g} = (1 - s_l)^2 \left(1 - s_l^2\right)$$

P=10MPa
T=200 C
CO_2 mol frac=0.7
Gas. Sat.=0.95

RUN-file (scenario 5)

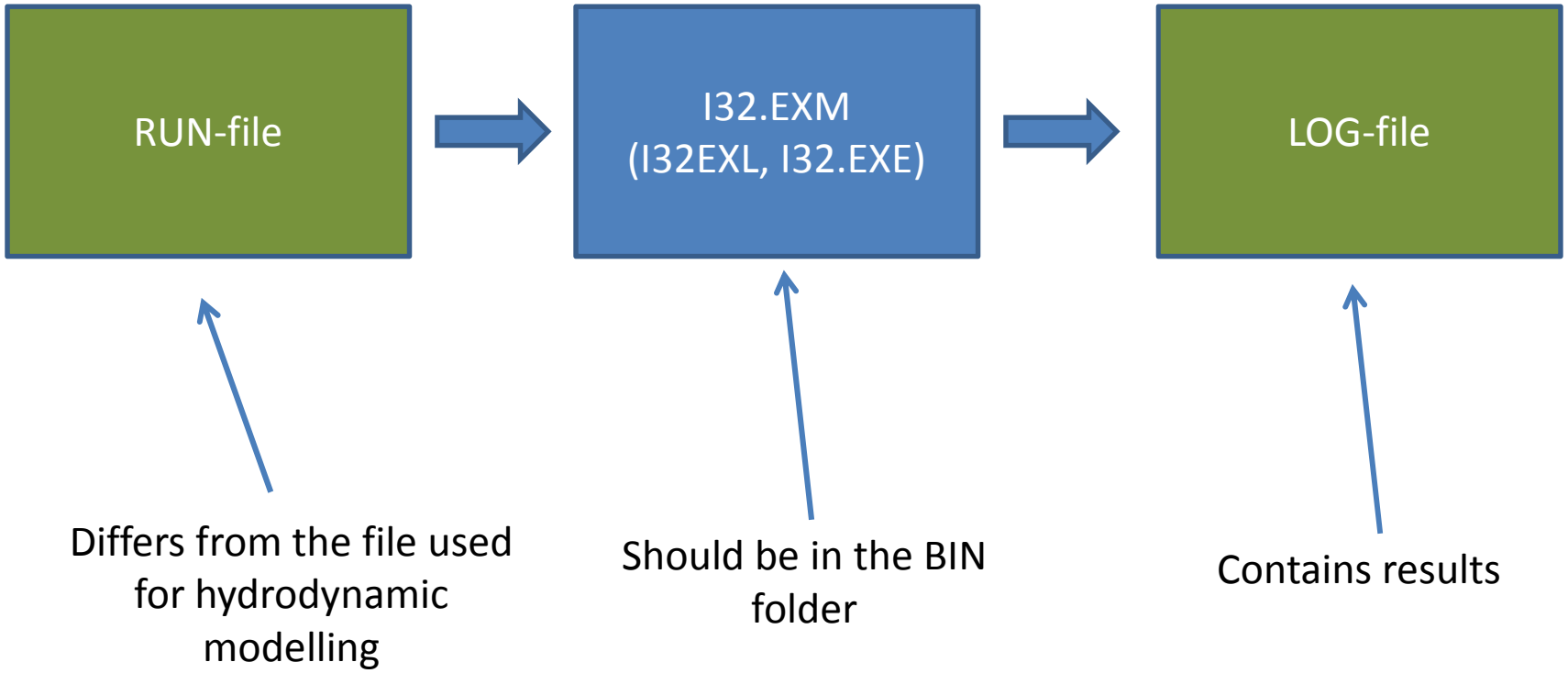
1. Open RUN-file in text editor
2. Run the simulation
3. Open results in ParaView

Result (scenario 5)



PVT program

PVT-program allows to calculate properties of the binary mixture for a given parameters (e.g., pressure, temperature, etc.). The calculation reports are outputted in LOG-file.



Properties for a given P and T

The properties for a given pressure, temperature and composition can be calculated by the **PHEQPTX** keyword.

PHEQPTX syntax

```
PHEQPTX
  pres1  temp1  comp1t1 comp2t1 /
  pres2  temp2  comp1t2 comp2t2 /
  pres3  temp3  comp1t3 comp2t3 /
  ...
/

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

  pres#   - pressure;
  temp#   - temperature (degrees of Kelvin);
  comp1t# - total molar fraction of the 1st component;
  comp2t# - total molar fraction of the 2nd component.
```

PVT program (exercise)

Exercise: Calculate thermodynamic equilibriums for initial conditions in Scenario 5:

1) PRES=10MPa, TEMPC=100C, COMP1T=0
2) PRES=10MPa, TEMPC=200C, COMP1T=0.7

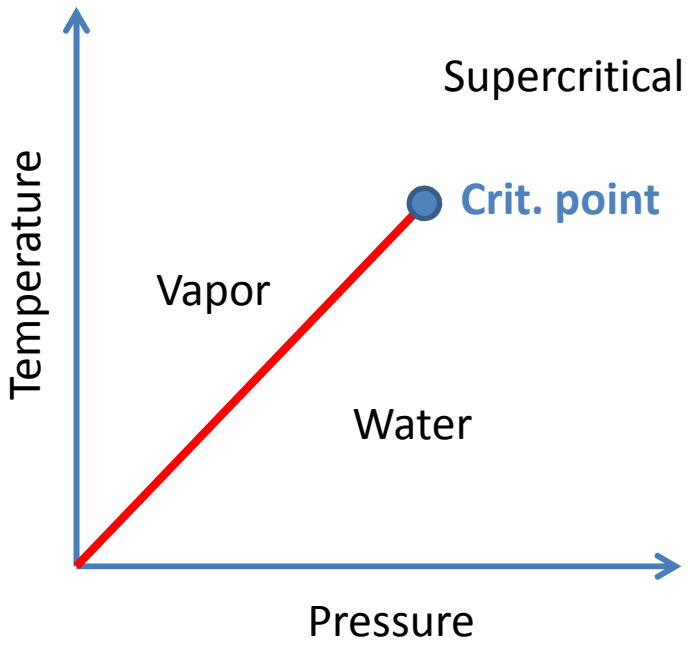
1. **Open RUN-file in text editor**
2. **Run the simulation**
3. **Open LOG-file to see results**

PHASES keyword

When moving around the critical point in the phase diagram there is no strict boundary between liquid phase and gaseous phase.

The PHASES keyword defines characteristic parameters of phases which can be used to output from hydrodynamic simulation the phases saturations, phases densities, viscosities etc.

Water phase diagram



PHASES keyword

PHASES syntax

```
-- in PROPS section

PHASES
   name1  pres1  entht1  comp1t1  comp2t1 /
   name2  pres2  entht2  comp1t2  comp2t2 /
   name3  pres3  entht3  comp1t3  comp2t3 /
   ...
/

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

   name#   - phase name (4-byte character);
   pres#   - pressure;
   entht#  - total molar enthalpy;
   comp1t# - total molar fraction of the 1st component;
   comp2t# - total molar fraction of the 2nd component.
```

Note, that the enthalpy for a phase definition can be calculated for a given temperature using PVT program.

The recommended parameters of phases (for H_2O subcritical conditions) are

- H_2O-rich phase: PRES= 1 MPa, ENTHT=5 kJ/mol, COMP1T=0
- CO_2-rich phase: PRES= 10 MPa, ENTHT=10 kJ/mol, COMP1T=1

PHASES keyword

The PHASES keyword creates the following mnemonics:

Mnemonic	Description
SAT#name	Saturation
DEN#name	Density
VIS#name	Viscosity
…	See Reference manual

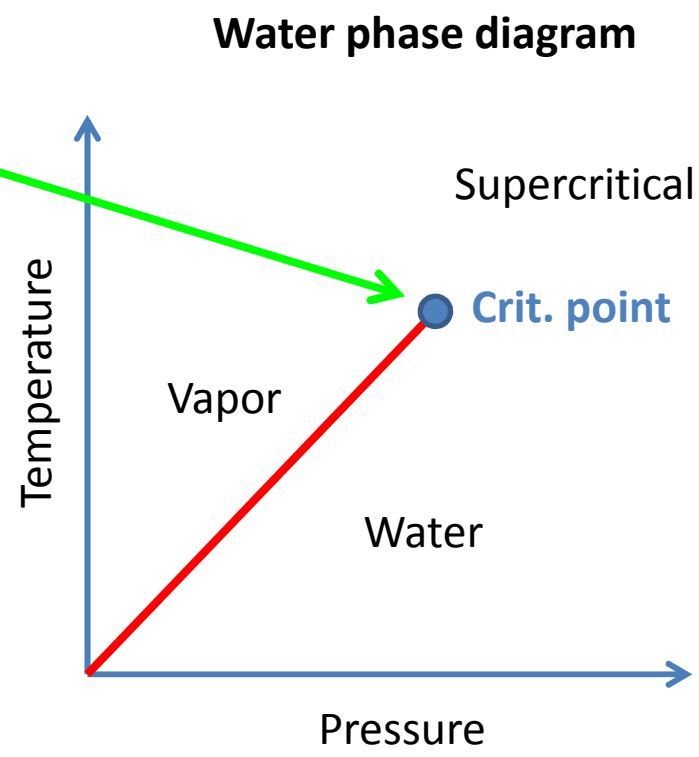
Here, ‘name’ is the phase name defined by the PHASES keyword.

Using BINMIXT module

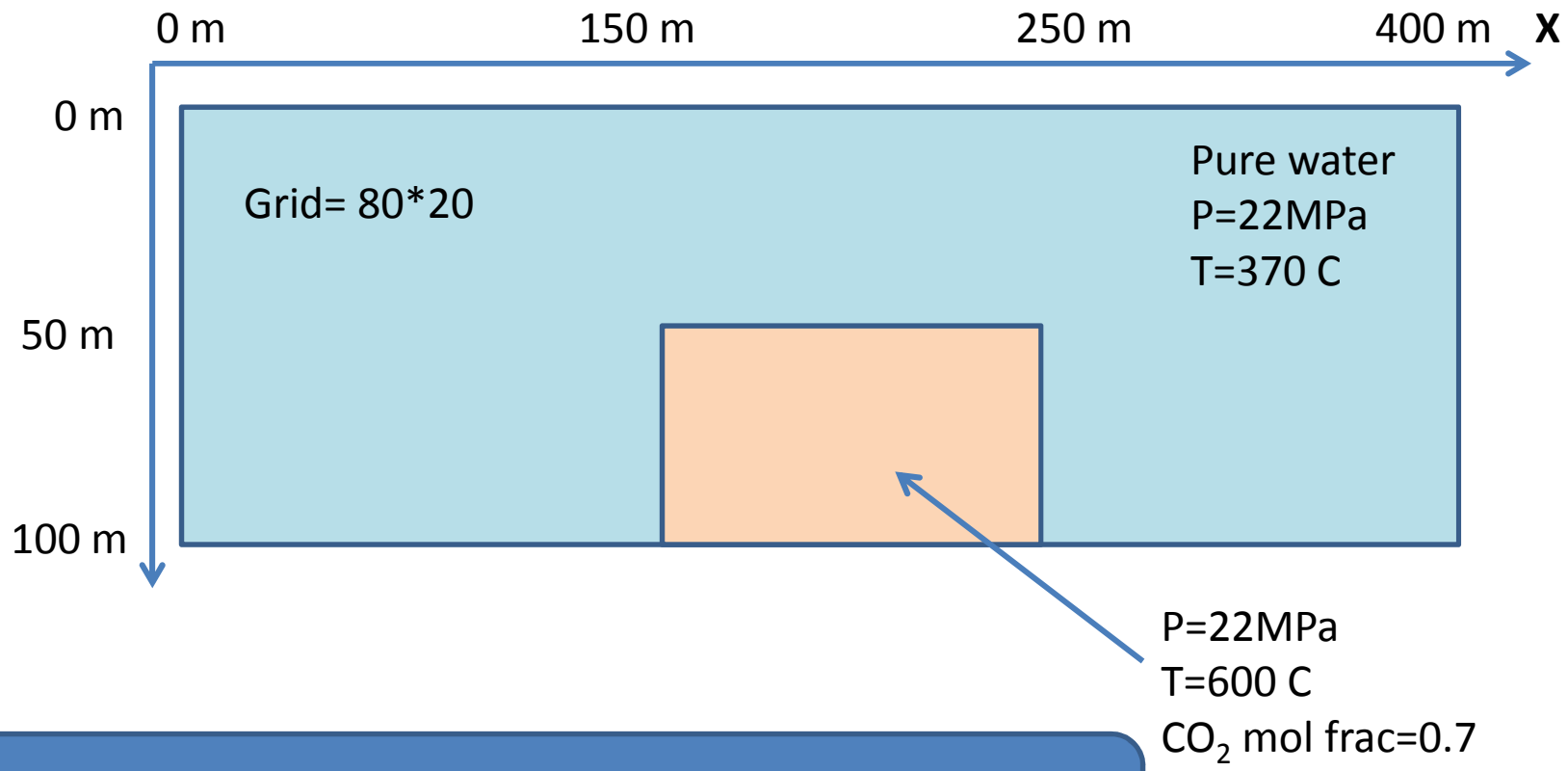
Exercise: Re-simulate scenario 5 saving in the summary files the saturations, densities and viscosities of phases.

Saturation functions scaling

The relative permeabilities must be linear function of saturation under critical conditions. The simulator can automatically scale the saturation functions defined by the keyword SATTAB under near critical conditions. This option is enabled by the SATCRT keyword.



Using BINMIXT module



Exercise: Re-simulate scenario 5 for new initial conditions

POST section

POST section

In the POST section the MUFITS output can be postprocessed to produce consolidated files, e.g., for time series data for grid blocks, point sources, wells etc.

Some of the available keywords are

Keyword	Description
POSTBLOC	Output parameters variations with time in grid blocks
POSTSRC	Output variation with time of point sources/sinks parameters
POSTWELL	Output variations with time of wells parameters

Keyword RPTPOST

The properties saved from the POST section are specified by the RPTPOST keyword. Note, that the program searches for these properties only in the summary files. Thus, these properties should be included in output from the SCHEDULE section, e.g., by the RPTSUM keyword.

RPTPOST syntax

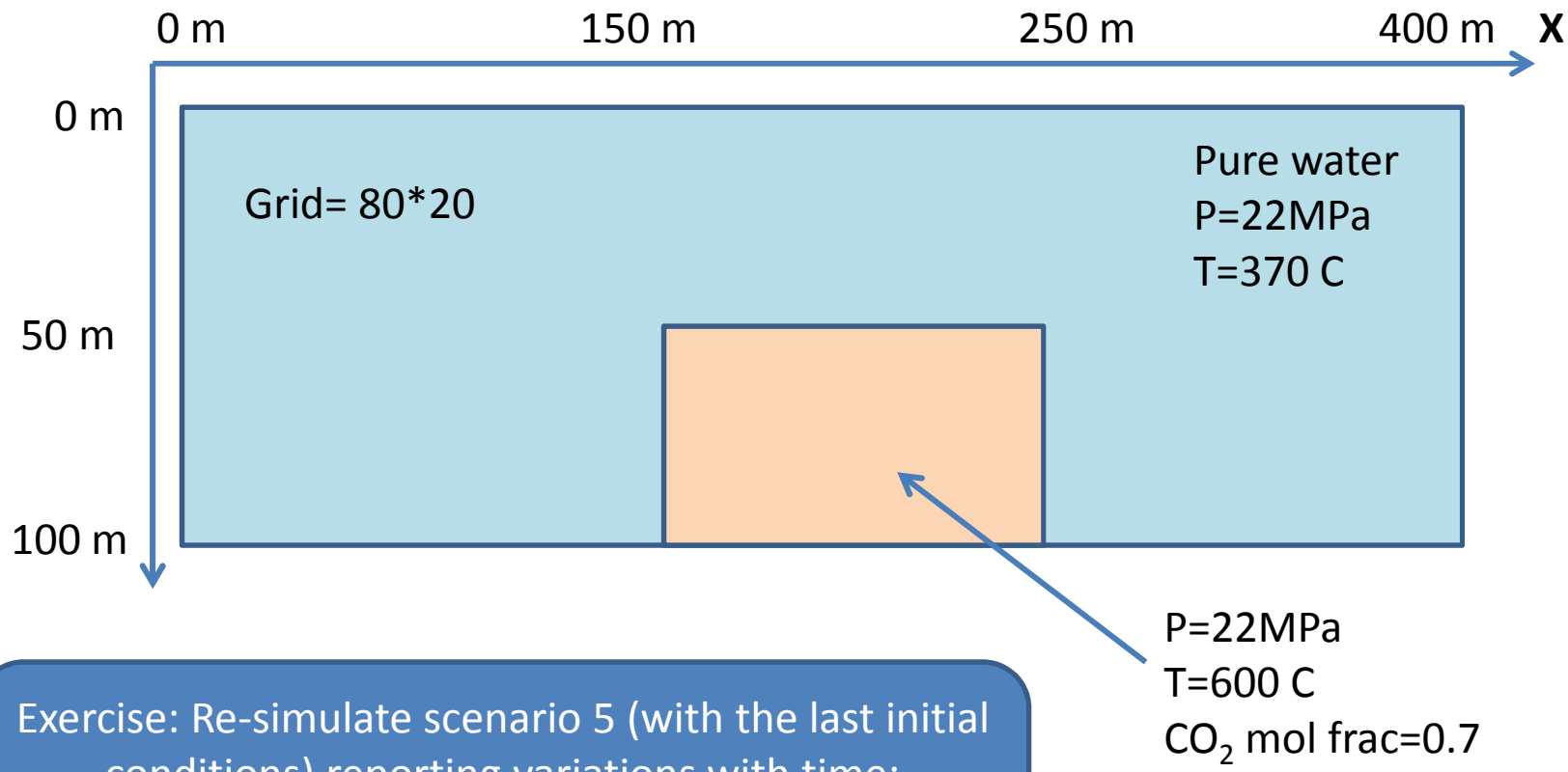
```
-- in POST section

RPTPOST
   mnemonic1  mnemonic2  mnemonic3  ...  /

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

      mnemonic# - is the mnemonic of a property saved from the POST section.
                  If one of the mnemonics is ASCII then the formatted file
                  is saved. If one of the mnemonics is ASCII then the binary
                  file is saved. If one of the mnemonics is NOTHING then the
                  output list is cleared.
```

Keyword POSTBLOC

POSTBLOC syntax

```
in POST section

POSTBLOC
   i1  j1  k1  gridname1  resname1  filename1 /
   i2  j2  k2  gridname2  resname2  filename2 /
   i3  j3  k3  gridname3  resname3  filename3 /
   ...
/

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

   i#        - i-index of the grid block;
   j#        - j-index of the grid block;
   k#        - k-index of the grid block;
   gridname# - grid name (e.g., defined by the CARFIN keyword);
   resname#  - reservoir name;
   filename# - output file name (if not specified the program uses default
               naming convention).
```

POST section (exercise)



Exercise: Re-simulate scenario 5 (with the last initial conditions) reporting variations with time:

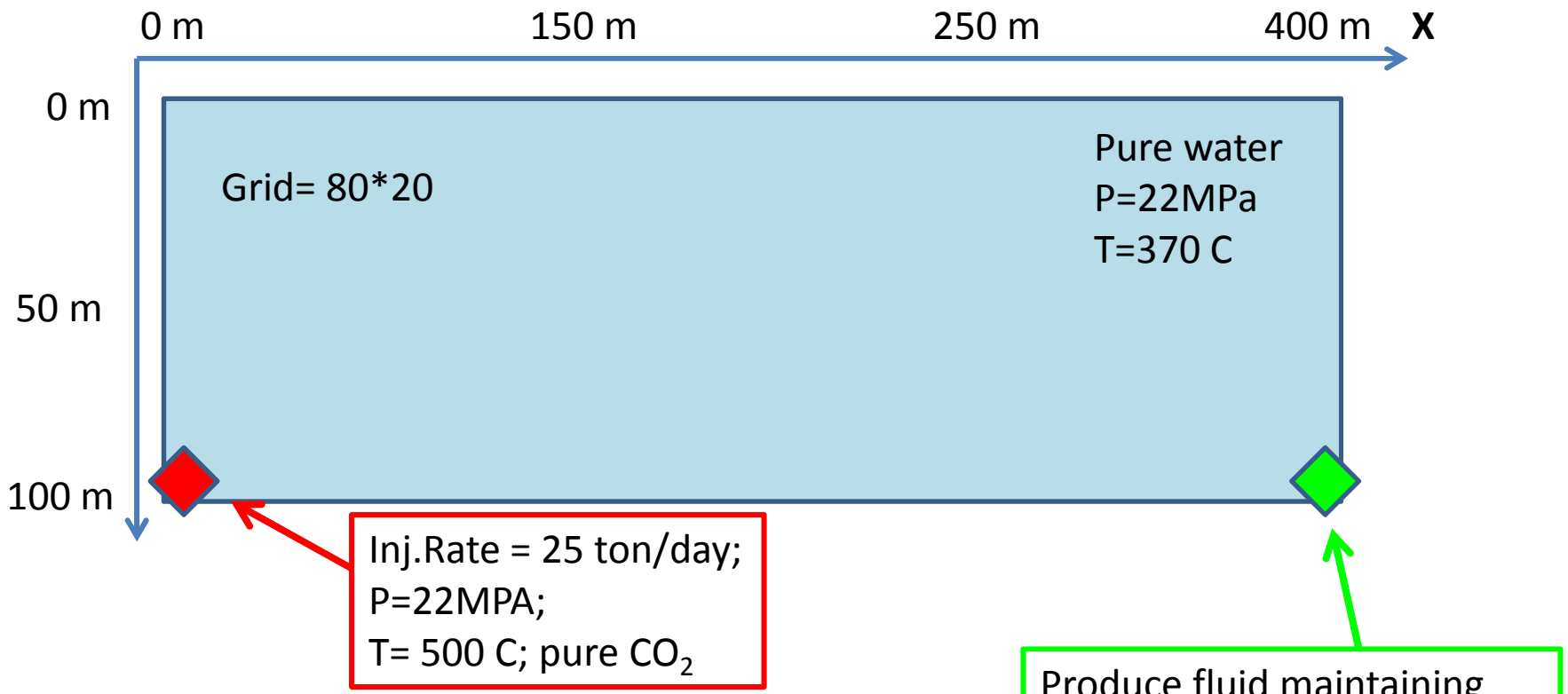
1) COMP1T, SAT#LH2O in block (31,1,3);
2) PRES and TEMPC, COMP1T in block (40,1,8).

Keyword POSTSRC

POSTSRC syntax

```
-- in POST section

POSTSRC
  srcname1  filename1 /
  srcname2  filename2 /
  srcname3  filename3 /
  ...
/

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

       srcname#  - the point source/sink name for which the output is required;
       filename# - output file name (if not specified the program uses default
                   naming convention).
```

POST section (exercise)



Exercise: Re-simulate scenario 5 introducing the point sources and reporting variation with time of the sources parameters. Plot the graphs in ParaView.

RUN-file (scenario 5; exercise)

1. Open RUN-file in text editor
2. Run the simulation
3. Open LOG-file to see results

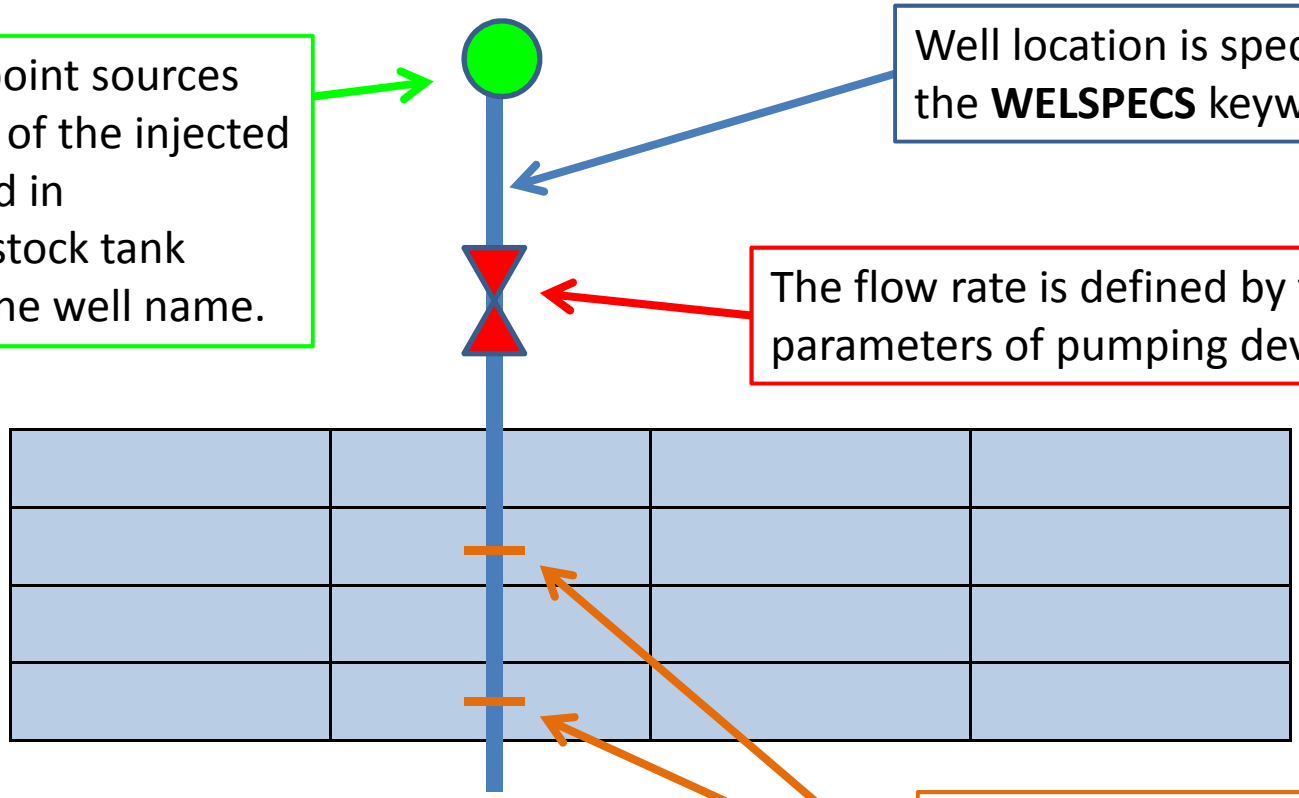
Wells

Some notes on wells

Like in case of point sources the parameters of the injected fluid are defined in corresponding stock tank referred to by the well name.

Well location is specified by the **WELSPECS** keyword

The flow rate is defined by the parameters of pumping device.



Well completions are specified by the **COMPDAT** keyword

The **WELSPECS** and **COMPDAT** keyword should be specified within **MAKE-ENDMAKE** brackets.

WELSPECS keyword

WELSPECS syntax

```
-- within MAKE-ENDMAKE brackets or in SCHEDULE section

WELSPECS
   name1 nu1 iloc1 jloc1 datum1 nu1 r0_1 3*nu1 eosnum1 5*nu1 fluxnum1 /
   name2 nu2 iloc2 jloc2 datum2 nu1 r0_2 3*nu2 eosnum2 5*nu2 fluxnum2 /
   name3 nu3 iloc3 jloc3 datum3 nu1 r0_3 3*nu3 eosnum3 5*nu3 fluxnum3 /
   ...
/

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

   name#    - well name;
   nu#      - a parameter not used at present;
   iloc#    - i-index of the grid block where the well head is located;
   jloc#    - j-index of the grid block where the well head is located;
   datum#   - reference depth for bottom hole pressure;
   r0_#     - drainage radius;
   eosnum#  - equation of state region number used for the fluid properties
              calculation in the well;
   fluxnum# - FLUXNUM region number assigned to all cells of which the well
              is constructed.
```

COMPDAT keyword

COMPDAT syntax

```
-- within MAKE-ENDMAKE brackets or in SCHEDULE section

COMPDAT
 name1 iloc1 jloc1 kmin1 kmax1 mode1 satnum1 tran1 d1 kh1 skin1 nu1 dir1 r0_1 /
 name2 iloc2 jloc2 kmin2 kmax2 mode2 satnum2 tran2 d2 kh2 skin2 nu2 dir2 r0_2 /
 name3 iloc3 jloc3 kmin3 kmax3 mode3 satnum3 tran3 d3 kh3 skin3 nu3 dir3 r0_3 /
 ...
/

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

   name#       - well name;
   nu#         - a parameter not used at present;
   iloc#/jloc# - i-index and j-index of the grid block where the well is
                 completed;
   kmin#/kmax# - k-index range of grid blocks where the well is completed;
   mode#       - if OPEN (default) the completion is opened for the fluid
                 transport; if SHUT the completion is closed off;
   satnum#     - saturation functions region (SATNUM) used for the calculation
                 of the fluxes through the completion;
   tran#       - this field is for explicit specification of the
                 transmissibility;
   d#          - wellbore diameter at the connection;
```

WELLPROD keyword

The parameters of production wells are specified using **WELLPROD** keyword

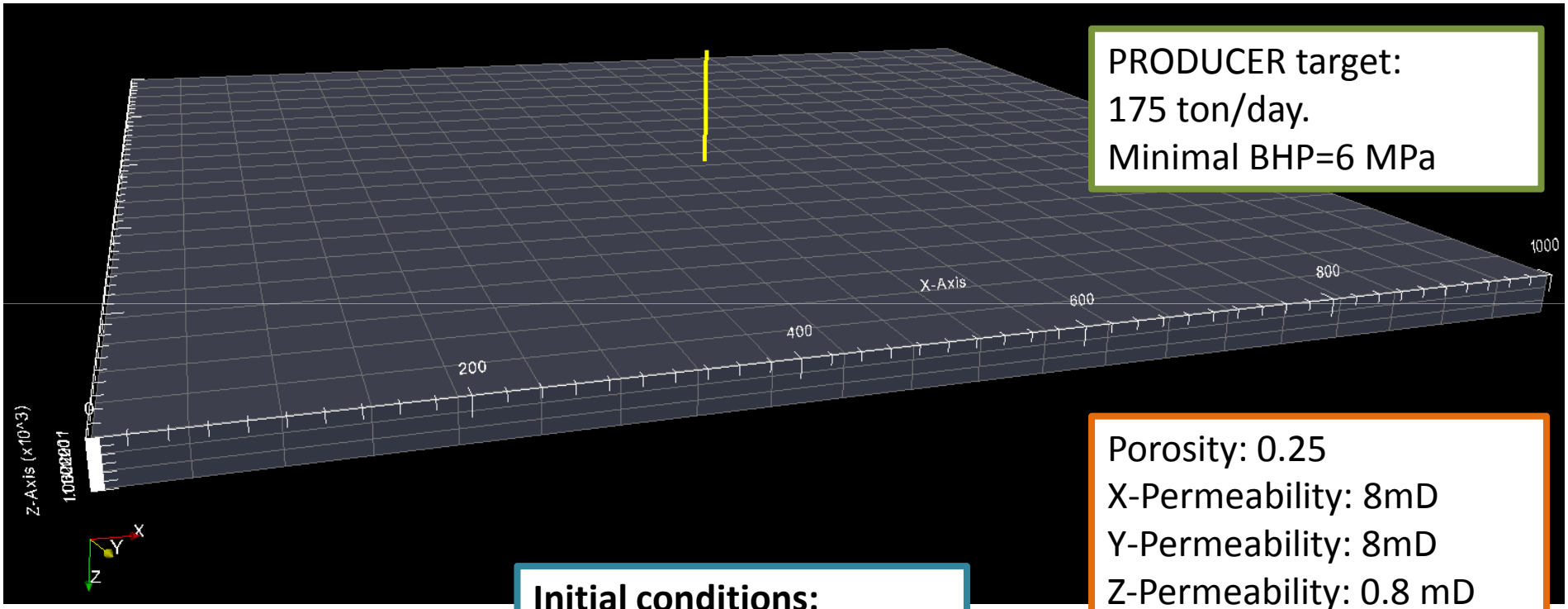
WELLPROD syntax

```
-- in SCHEDULE section

WELLPROD
   name1 mode1 targ1 volrate1 massrate1 bhp1 vp1 nu1 dimflag1 /
   name2 mode2 targ2 volrate2 massrate2 bhp2 vp2 nu2 dimflag2 /
   name3 mode3 targ3 volrate3 massrate3 bhp3 vp3 nu3 dimflag3 /
   ...
/

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

   name#     - well name or well name template;
   mode#     - well mode. Available values: OPEN - well open for flow (default),
               STOP - well stoped above formation, SHUT - well completely
               isolated form the formation.
   targ#     - well operational target. Available values: MASS - mass rate,
               RESV - volumetric rate at reservoir conditions, BHP - constant
               bottom hole pressure;
   massrate# - mass rate;
   volrate#  - volumetric rate;
   bhp#      - bottom-hole pressure (either limit (MASS,RESV) or target
               parameter (BHP));
```

Scenario 6

Grid: 21*21*3
Domain:[0,1000]*[0,1000]*[1000,1030] m
PRODUCER: i=11, j=11 completed in k=1,2

Simulate production for 9540 days reporting distributions every 180 days. Create plots for well flow rate, bottom-hole pressure and bottom-hole temperature.



PRODUCER target:
175 ton/day.
Minimal BHP=6 MPa

Porosity: 0.25
X-Permeability: 8mD
Y-Permeability: 8mD
Z-Permeability: 0.8 mD
HeatCondCoef: 2W/m/K
RockDens: 2650 kg/m3
RockHeatCapac: 1 kJ/kg/K

Initial conditions:
Temperature=307.8 C;
Equilibrium conditions;
Water saturation = 1.0

$$k_{r,l} = s_l^3$$

$$k_{r,g} = \left(1 - s_l\right)^2$$

RUN-file (scenario 6)

1. Open RUN-file in text editor
2. Run the simulation
3. Open LOG-file to see results

WELLINJE keyword

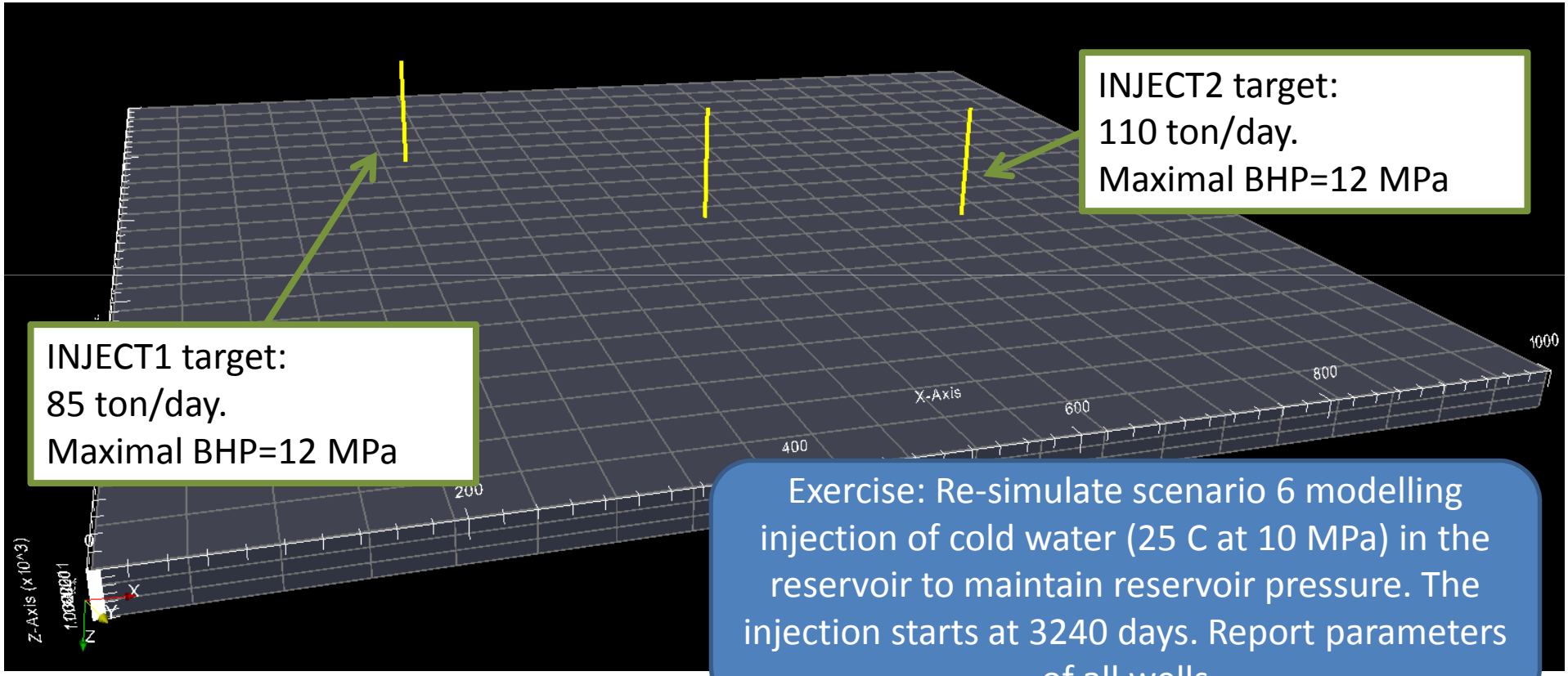
The parameters of injection wells are specified using **WELLINJE** keyword

WELLINJE syntax

```
-- in SCHEDULE section

WELLINJE
   name1 mode1 targ1 volrate1 massrate1 bhp1 vp1 injtype1 dimflag1 /
   name2 mode2 targ2 volrate2 massrate2 bhp2 vp2 injtype2 dimflag2 /
   name3 mode3 targ3 volrate3 massrate3 bhp3 vp3 injtype3 dimflag3 /
   ...
/

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

   name#     - well name or well name template;
   mode#     - well mode. Available values: OPEN - well open for flow (default),
               STOP - well stoped above formation, SHUT - well completely
               isolated form the formation.
   targ#     - well operational target. Available values: MASS - mass rate,
               RATE - volumetric rate at stock tank conditions, BHP - constant
               bottom hole pressure;
   massrate# - mass rate;
   volrate#  - volumetric rate;
   bhp#      - bottom-hole pressure (either limit (MASS,RATE) or target
               parameter (BHP));
```

Scenario 6 (exercise 1)

PRODUCER: i=11, j=11 completed in k=1,2
INJECT1: i=6, j=6 completed in k=1,2,3
INJECT2: i=16, j=12 completed in k=1,2,3



INJECT2 target:
110 ton/day.
Maximal BHP=12 MPa

INJECT1 target:
85 ton/day.
Maximal BHP=12 MPa

Exercise: Re-simulate scenario 6 modelling injection of cold water (25 C at 10 MPa) in the reservoir to maintain reservoir pressure. The injection starts at 3240 days. Report parameters of all wells

RUN-file (scenario 6; exercise 1)

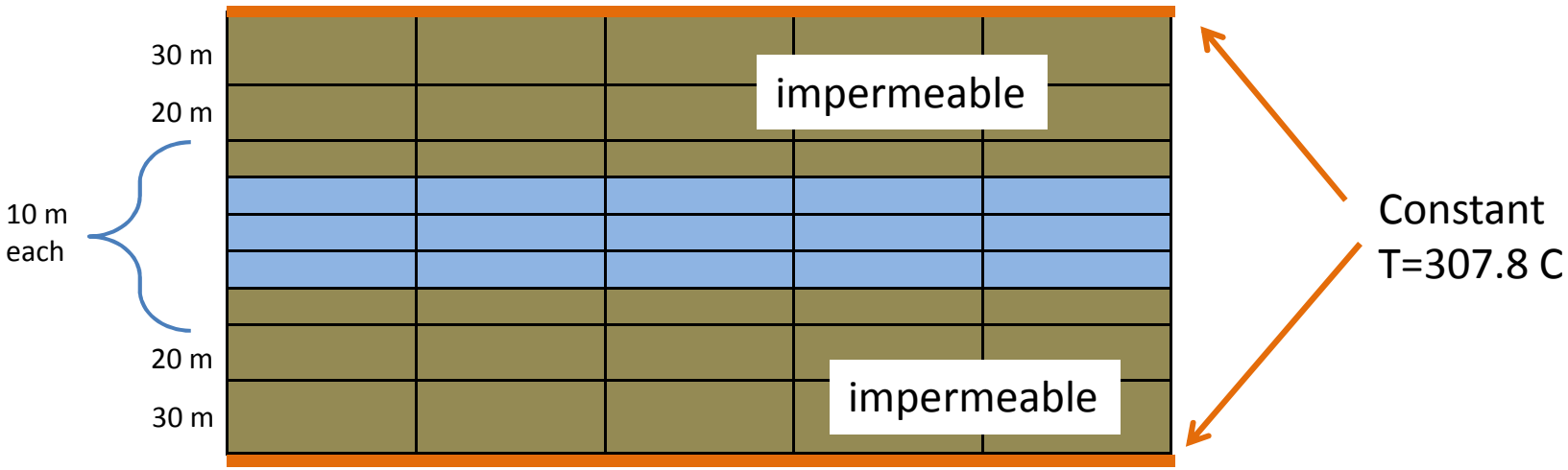
1. Open RUN-file in text editor
2. Run the simulation
3. Open LOG-file to see results

Scenario 6 (exercise 2)

Grid: 21*21*9

Exercise: Re-simulate scenario with 3 wells modelling heat exchange with impermeable overburden and underburden layers.

Cross-section view



RUN-file (scenario 6; exercise 2)

1. Open RUN-file in text editor
2. Run the simulation
3. Open LOG-file to see results

Scenario 6 (exercise 3)

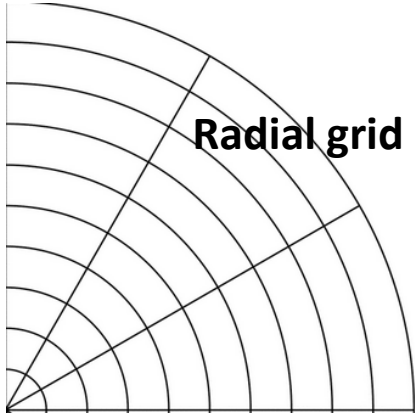
Exercise: Re-simulate Scenario 6 (exercise 2)
using EOS-module BINMIXT.
Use the following initial conditions in the reservoir
Pressure=9.577
Temperature=307.8 C
CO_2 mol.fraction=0.1

RUN-file (scenario 6; exercise 3)

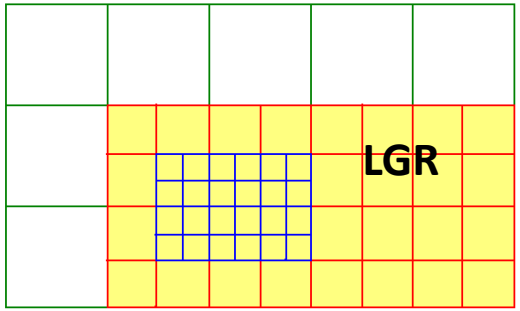
1. Open RUN-file in text editor
2. Run the simulation
3. Open LOG-file to see results

Next day

- Radial grids
- Fluid-in-place regions
- Local grid refinements
- Grid decomposition



$$A = \int_{domain} a \mathrm{d}V$$



Simulation is parallel using 1 core, 2 cores, 3 cores, … How the simulation is decomposed between the cores?