CO_2QUEST

Reactive transport simulations of an impure CO_2 flue gas injection into a saline aquifer on a 2D reservoir scale

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Impact of the Quality of CO_2 on Storage and Transport

effect of typical impurities in the CO_2 stream captured from fossil fuel power plants

- **safe and economic transportation**
- **deep geologic storage**

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To obtain an understanding of the effects of impurities on the performance of the geological storage operation, in terms of fluid/rock interactions and leakage of trace elements by means of:

1. **field injection tests of CO_2 with impurities (Heletz, Israel and Catenoy, France)**
2. **laboratory experiments to determine the impact of the impurities on the mechanical properties of the reservoir and the caprock**
3. **extensive model development and application to enhance the understanding of CO_2 geological storage performance in the presence of impurities**

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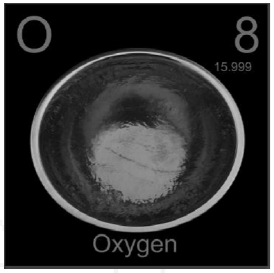
impact of impurities

physics

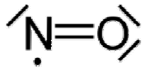
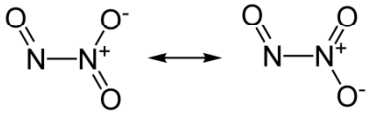
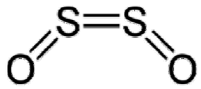
impact of non-condensible gases

- changing physical properties of CO_2
  mobility, density, wettability
  → injectivity

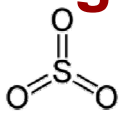
- use of pore space
  → smaller storage volume for CO_2



periodictable.com/Elements

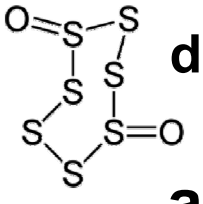
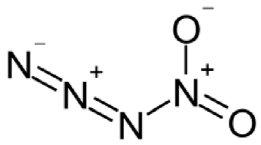





impact of chemically active gases – H_2S, NO_x, SO_x



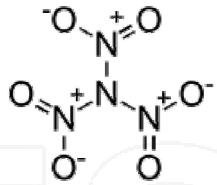
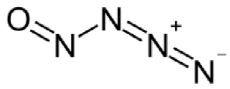
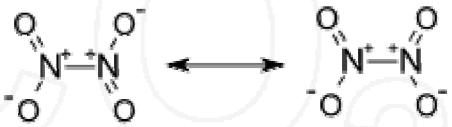
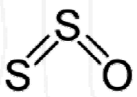
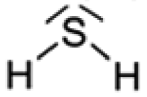
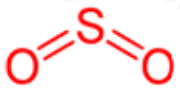
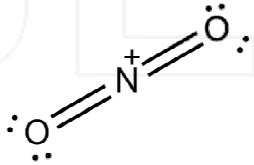

- **acidification around the well**

  dissolution of carbonates

- **acidification in greater distances**

  precipitation of secondary minerals

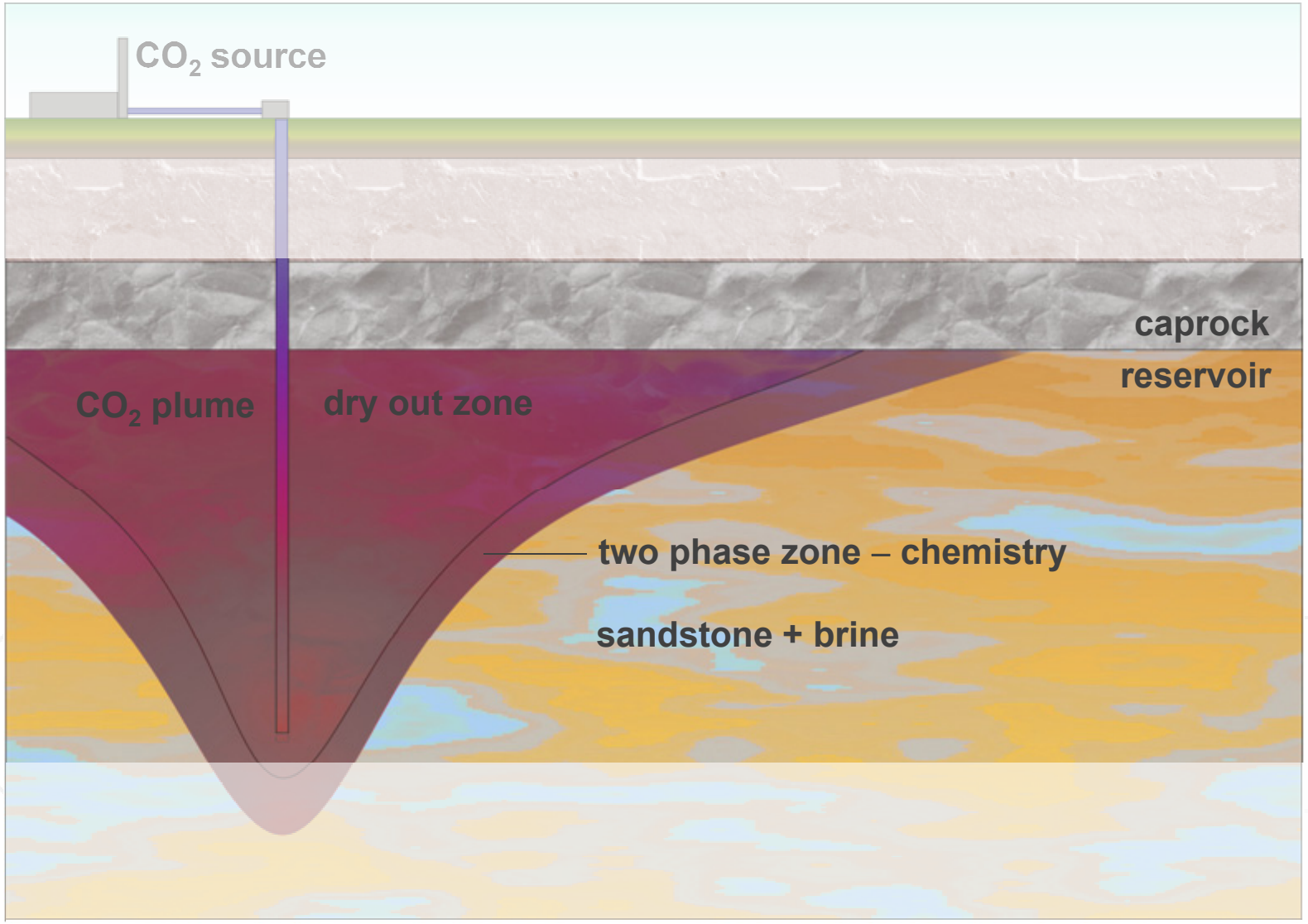








S=O

de.wikipedia.org/

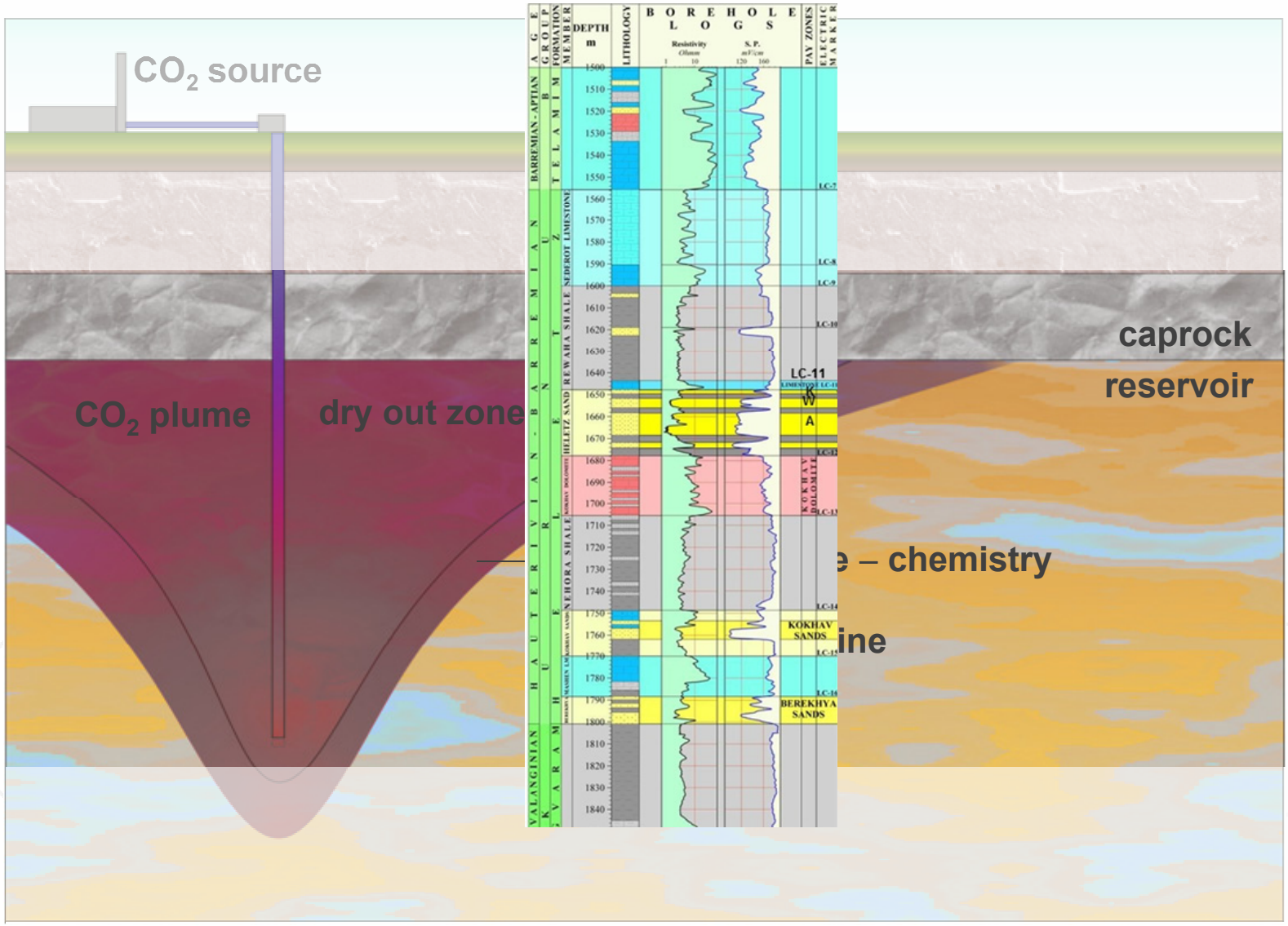
impact of impurities

reservoir



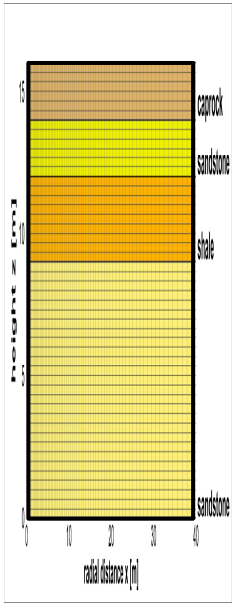
impact of impurities

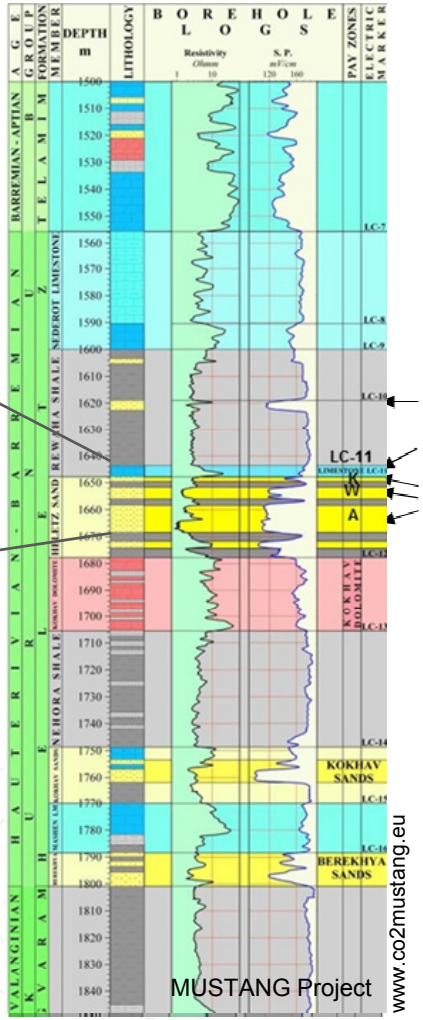
Heletz



2D radial model

initial





caprock, shales + marls

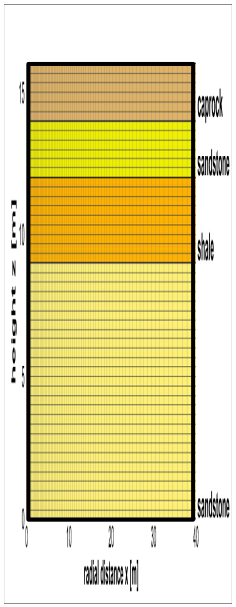
limestone layer LC11

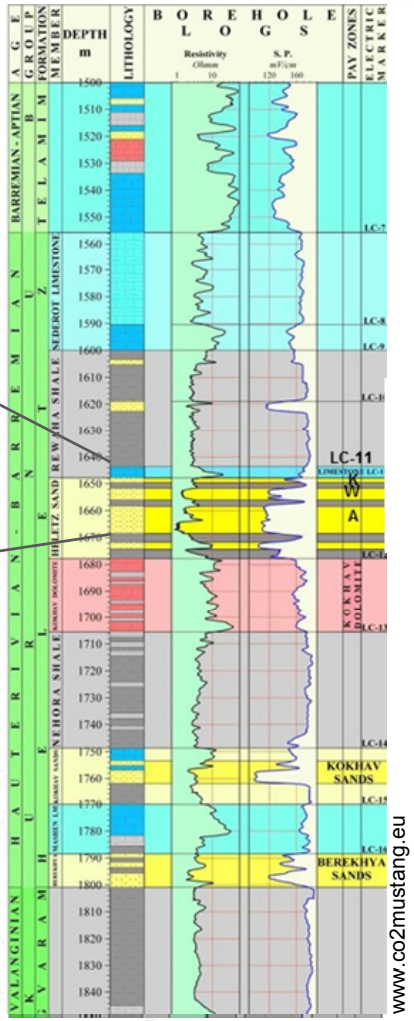
3 sand reservoir layers K, W, A

parameter	value
pressure	14.7 MPa
temperature	66 °C, isothermal
porosity	20 %
horizontal permeability	100 mD
vertical permeability	700 mD
thickness	18 m
rock density	2870 kg/m^3
salinity	0.055

2D radial model

minerals





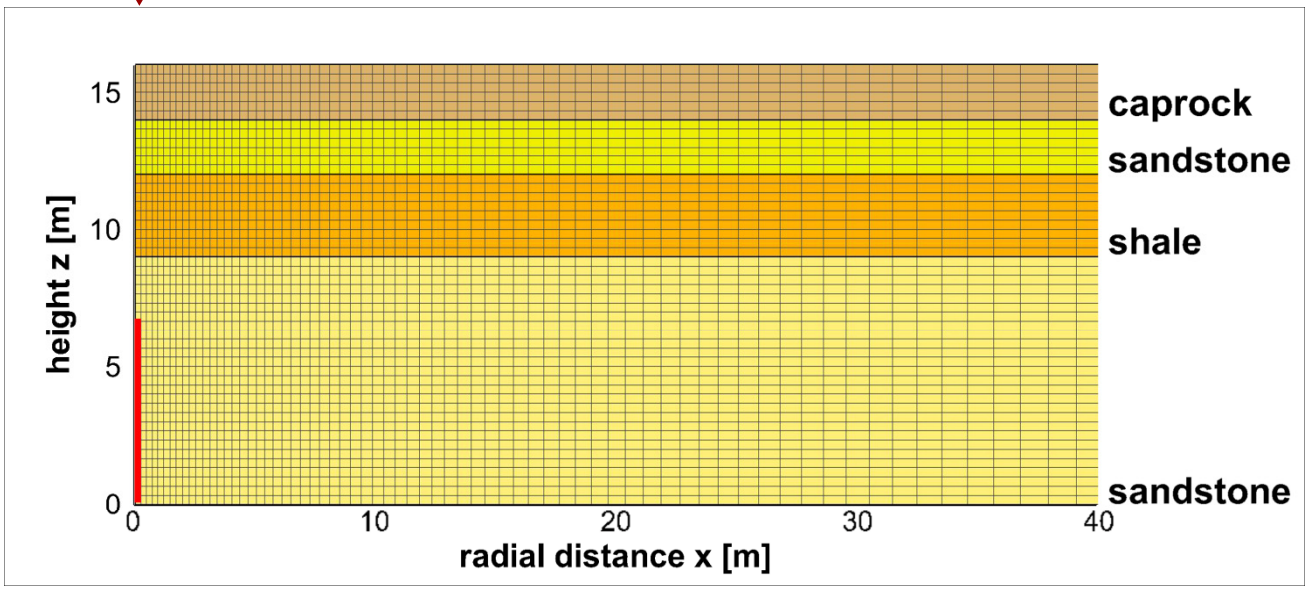
primary minerals	fraction
carbonates	
ankerite $CaFe_{0.7}Mg_{0.3}(CO_3)_2$	3.7 %
feldspars	
K-feldspar $KAlSi_3O_8$	12 %
albite $NaAlSi_3O_8$	3.9%
clay minerals	
illite $K_{0.85}Al_{2.85}Si_{3.15}O_{10}(OH)_2$	3.9 %
kaolinite $Al_2Si_2O_5(OH)_4$	3.2 %
chlinochlore-7a $Mg_5Al_2Si_3O_{10}(OH)_8$	1.4 %
sulfur minerals	
pyrite FeS_2	2.1 %
anhydrite $CaSO_4$	0.4 %
oxide mineral	
quartz SiO_2	69.35 %
iron mineral	
goethite FeOOH	0.05 %

secondary minerals	
carbonates	
calcite $CaCO_3$	
siderite $FeCO_3$	
iron mineral	
hematite Fe_2O_3	

2D radial model

injection

$CO_2 + SO_2$

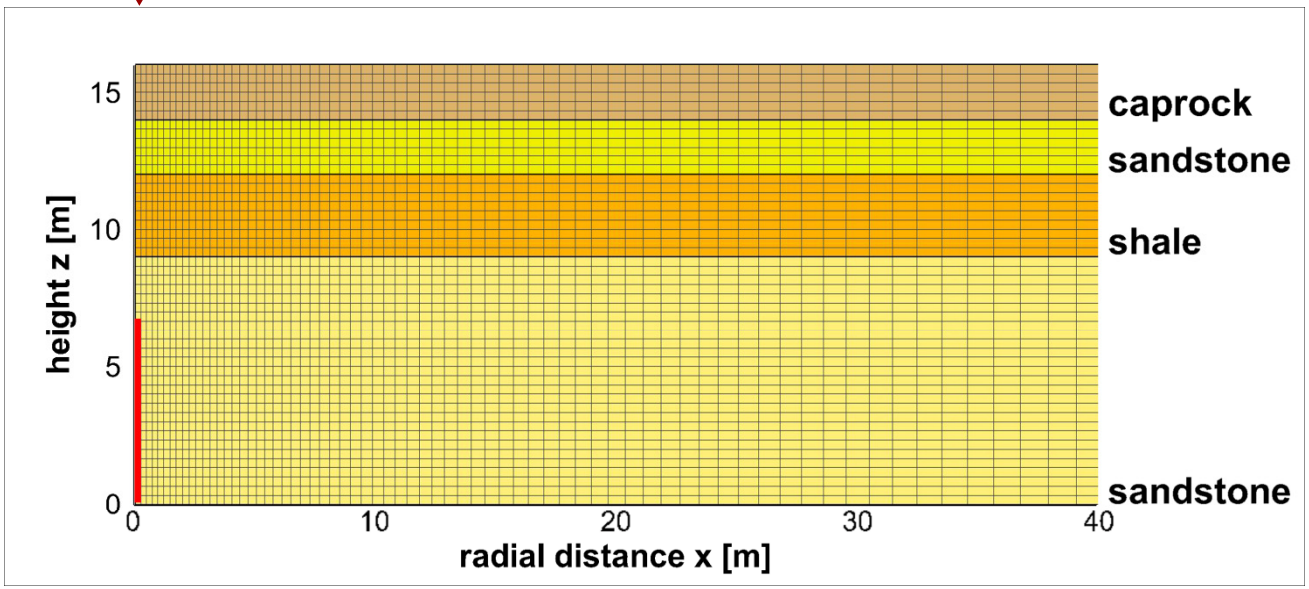


$scCO_2 + SO_2$
9 kg/s
0.28 Mt for 10 years
99:1

2D radial model

grid

$CO_2 + SO_2$



10710 cells in total

2D radial symmetric

x = 30000 m

x < 2000 m
220 cells
0.22 m < Δx < 49 m

x > 2000 m
30 cells

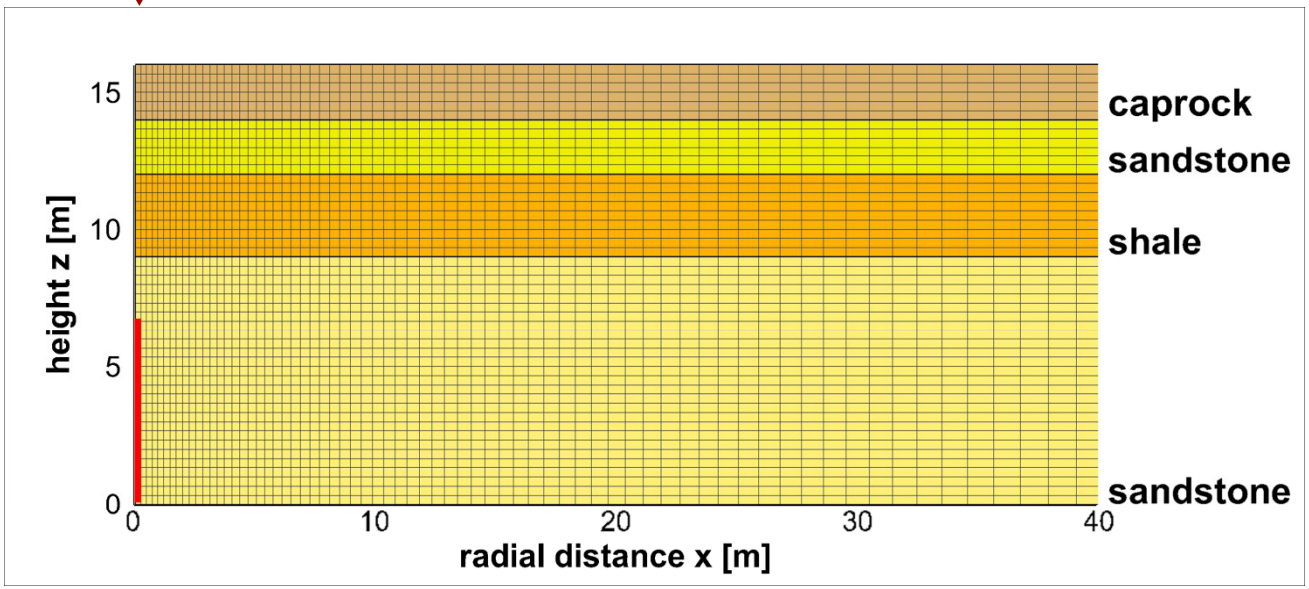
y = 16 m

x < 2000 m
48 cells

x > 2000 m
5 cells

2D radial model grid

$CO_2 + SO_2$



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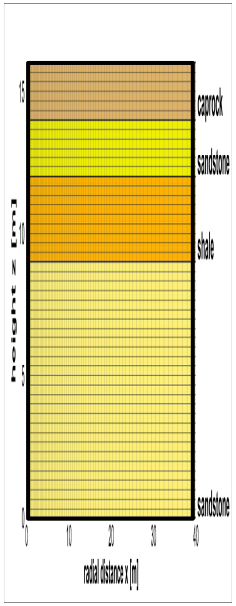
2D radial model

initial



caprock

sandstone

shale

sandstone

2D radial symmetric

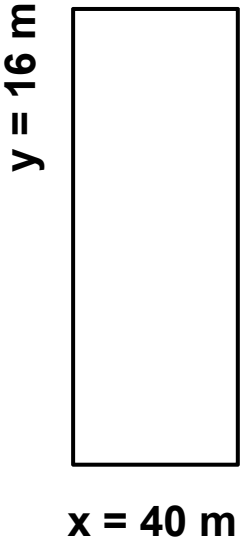
x = 30000 m

first 40 m shown

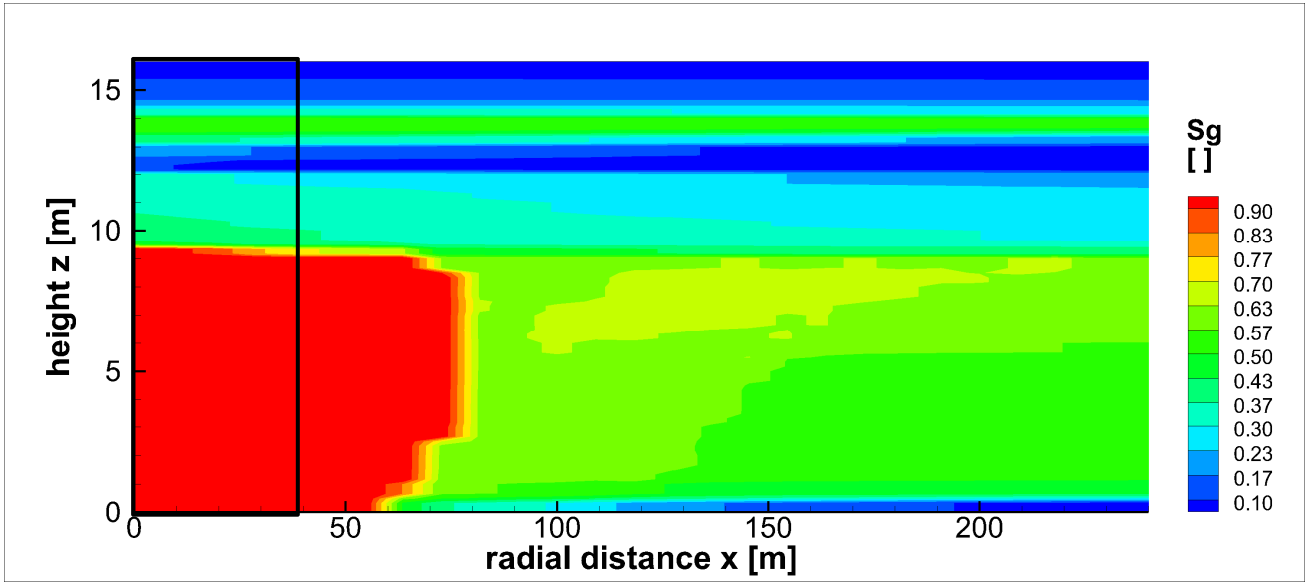
layer	height [m]	porosity [%]	horizontal permeability [mD]	vertical permeability [mD]	quartz [%]	feldspar [%]	clay minerals [%]	carbonates [%]	other minerals [%]
caprock	2	9.5	0.1	0.1	3	50	35	8	4
sandstone	2	21.3	700	100	70	16	8	4	2
shale	3	9.5	0.1	0.1	3	50	35	8	4
sandstone	9	15.6	700	100	70	16	8	4	2

reactive transport

grid



gas saturation Sg



2D radial symmetric

x = 30000 m

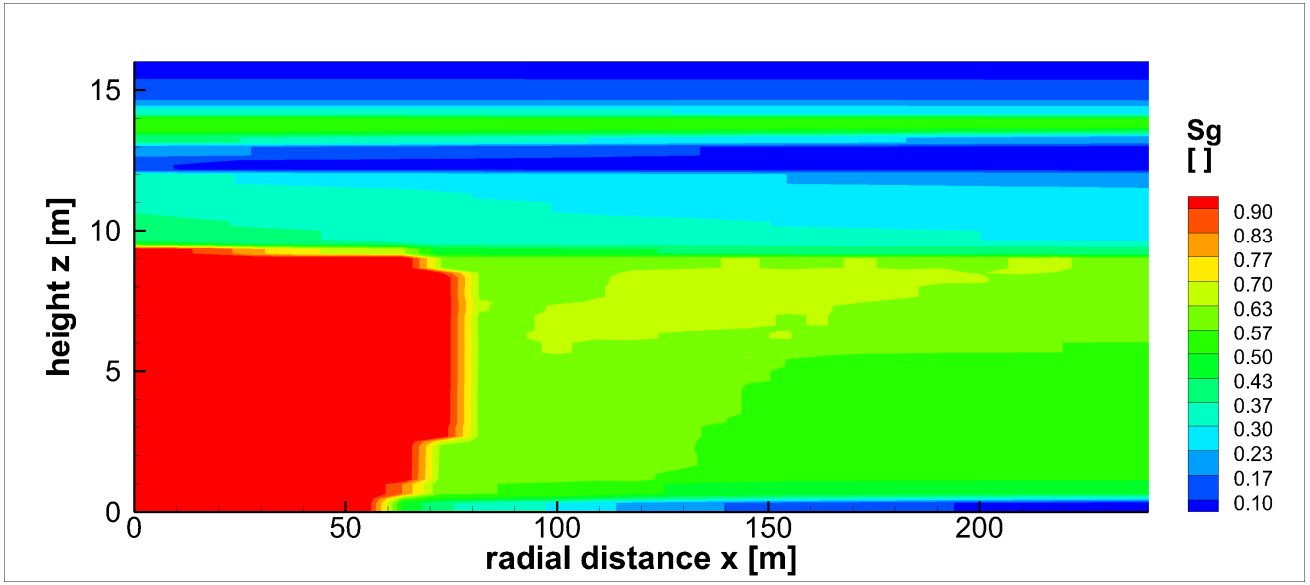
t = 10 a

shown

x = 240 m

TOUGHREACT V3-OMP, ECO2N

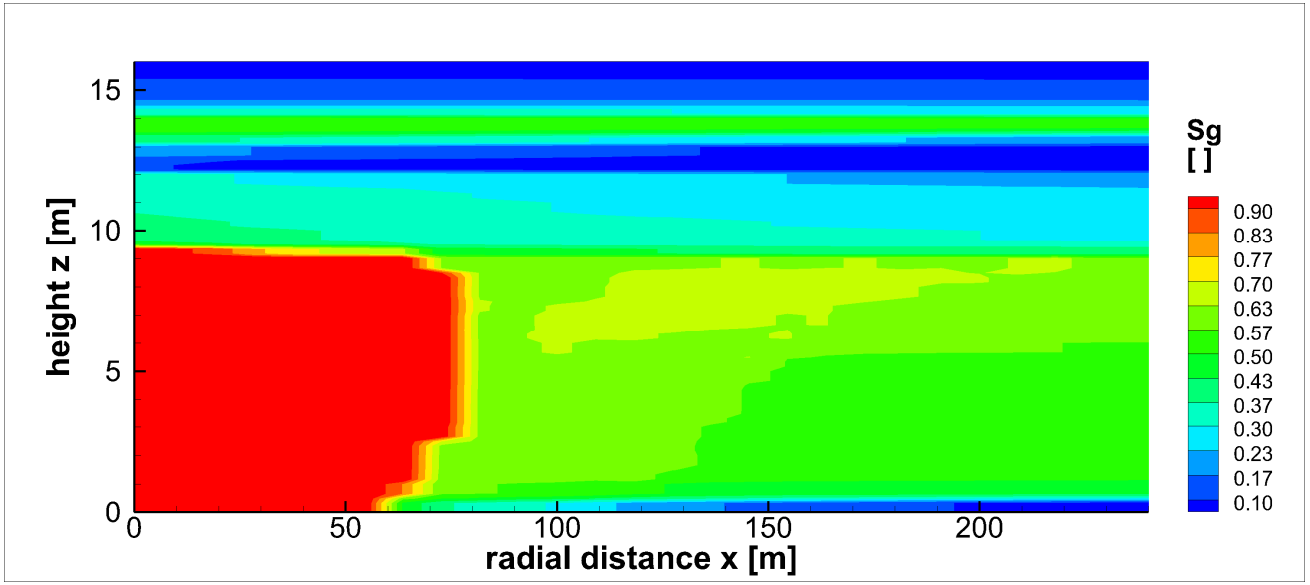
gas saturation Sg



CO_2 plume

x < 60 m
dry out zone

gas saturation Sg



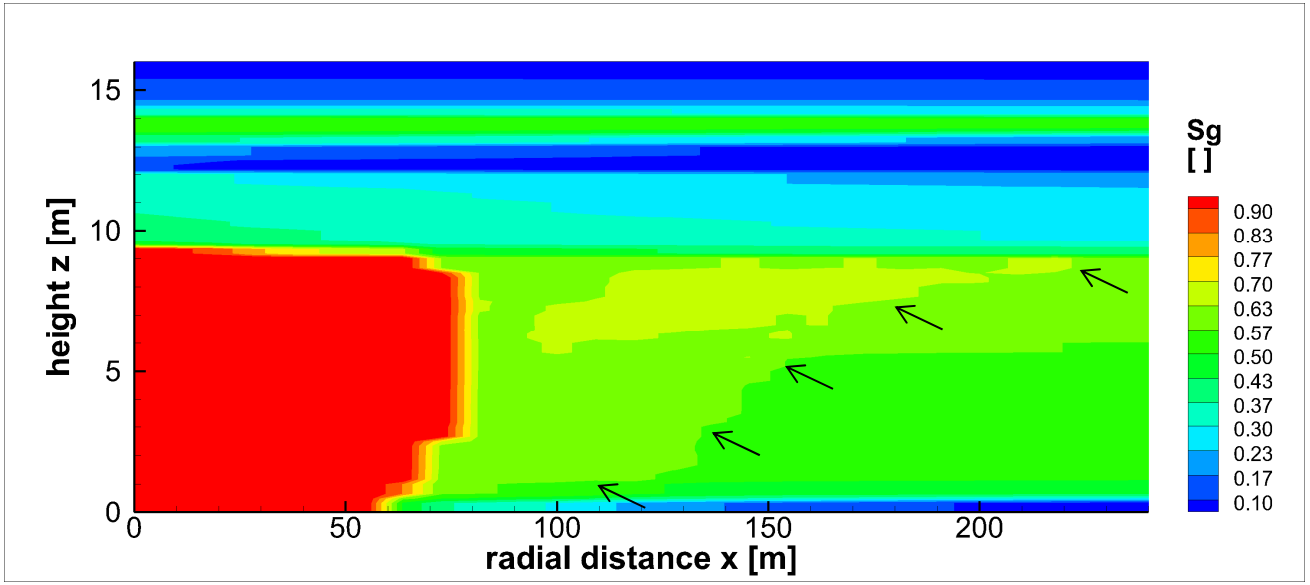
CO_2 plume

x < 60 m
dry out zone

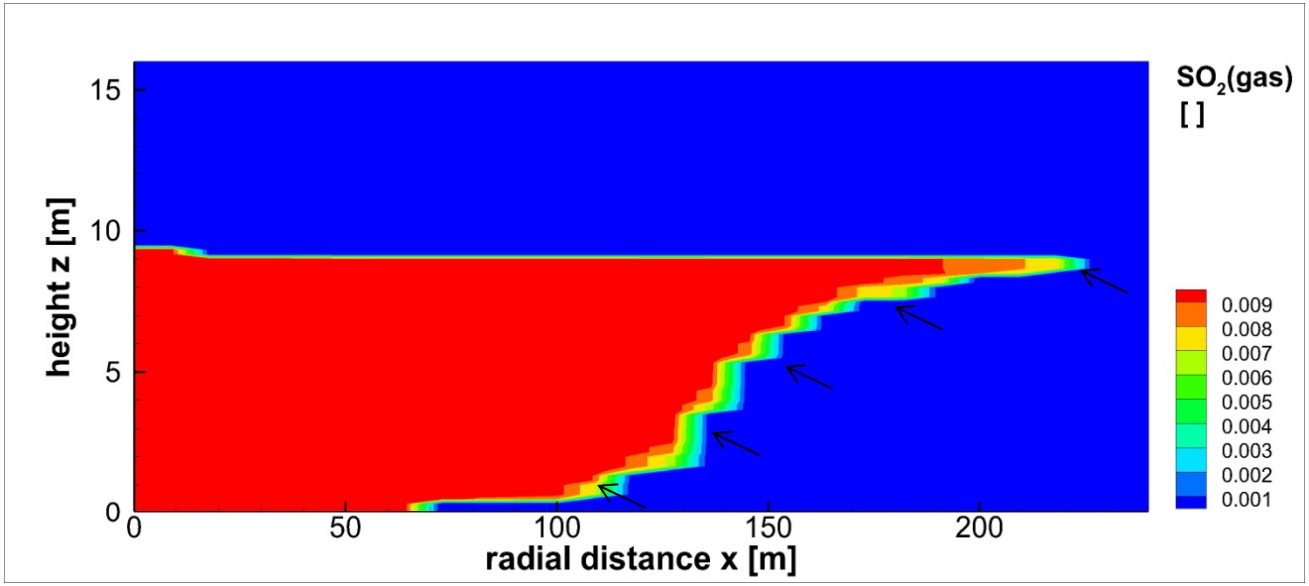
x < 400 m
influence of nearly whole sandy layer

x = 2500 m
maximum distance, lowest sandstone layer,
just below shale

gas saturation Sg

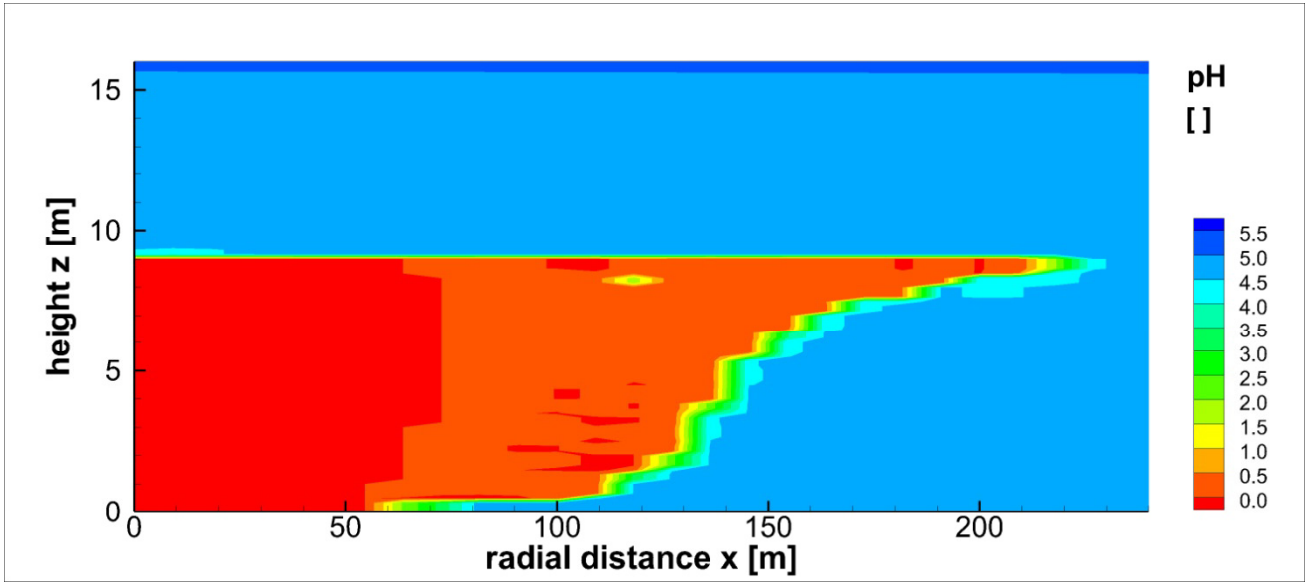


SO_2 (gas)



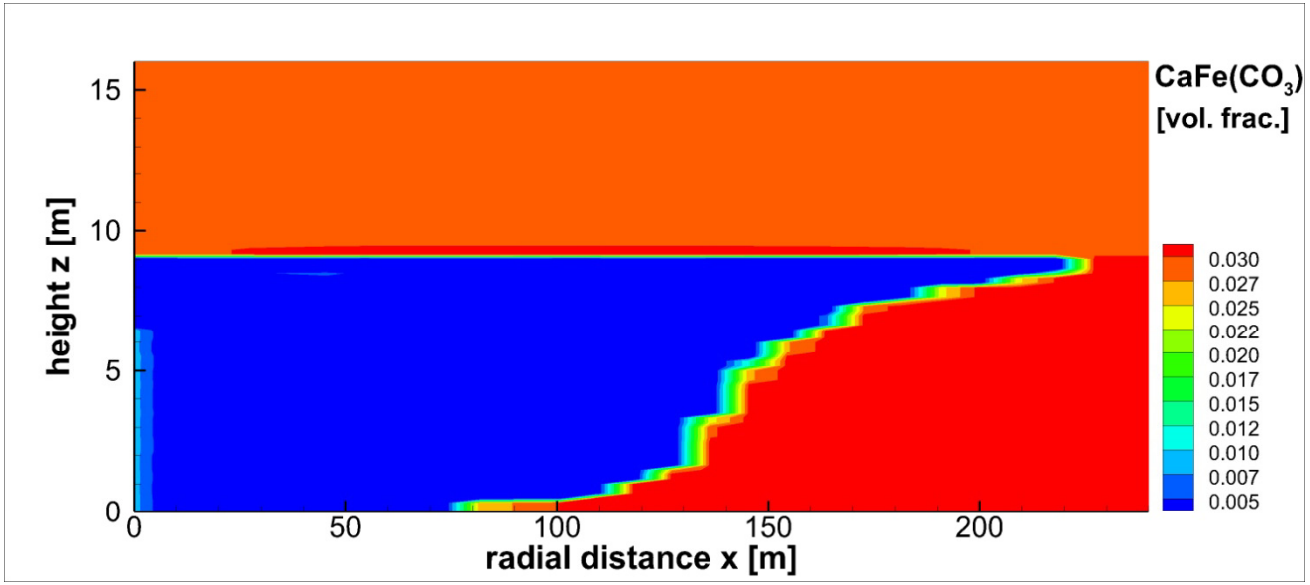
dry out zone just below shale layer

pH



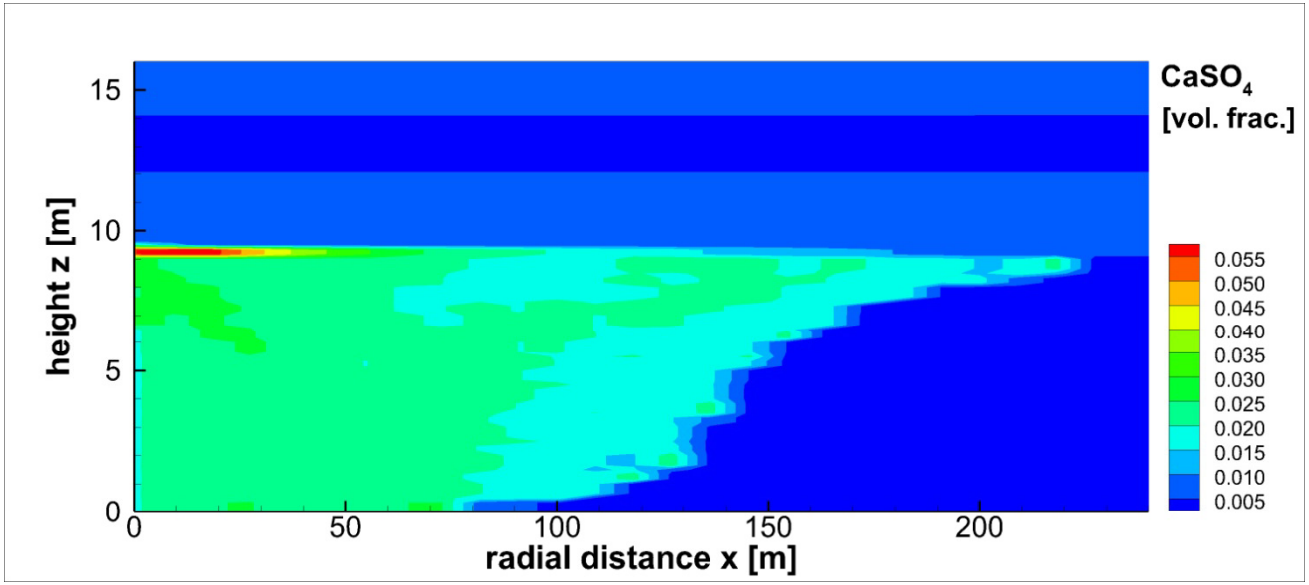
SO_2 influences pH

ankerite dissolved



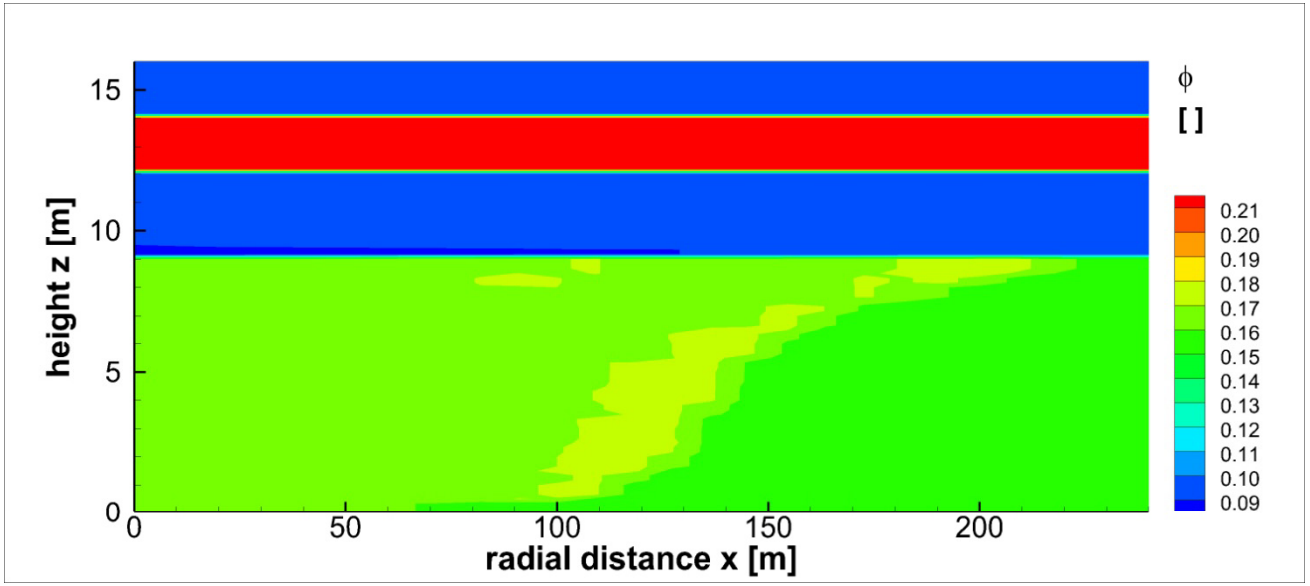
drop in pH influences carbonates

anhydrite precipitates



as
ankerite dissolves
anhydrite precipitates

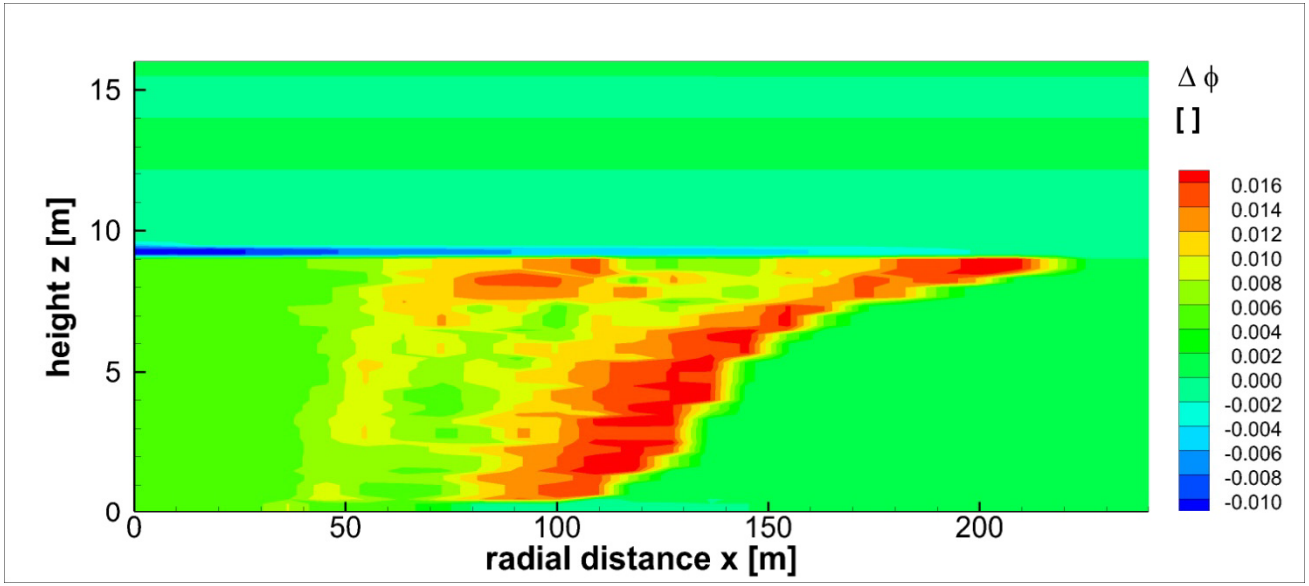
porosity



initial values

caprock	9.5 %
sandstone	21.3 %
shale	9.5 %
sandstone	15.6 %

change of porosity



molar volume

$CaCO_3$ 37 cm^3/mol
$CaSO_4$ 46 cm^3/mol

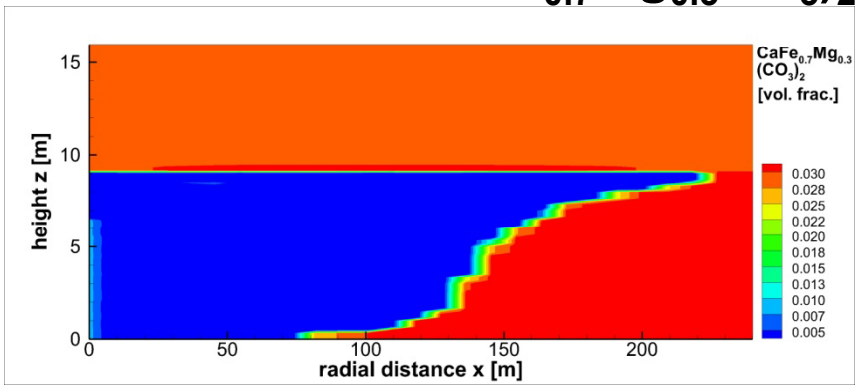
increase in ϕ

complex chemistry

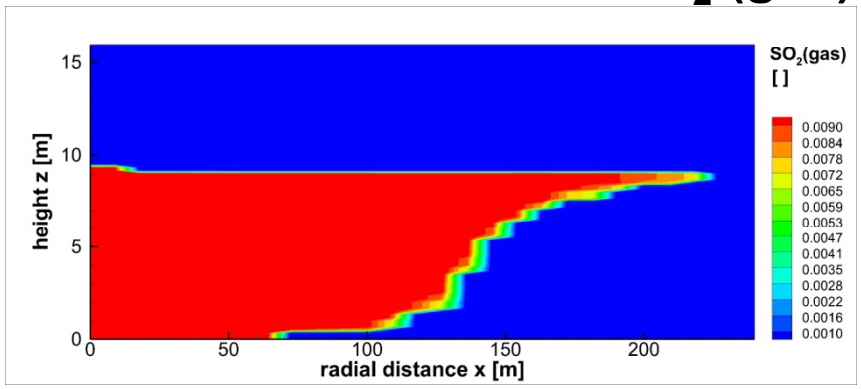
reactive transport

Ca

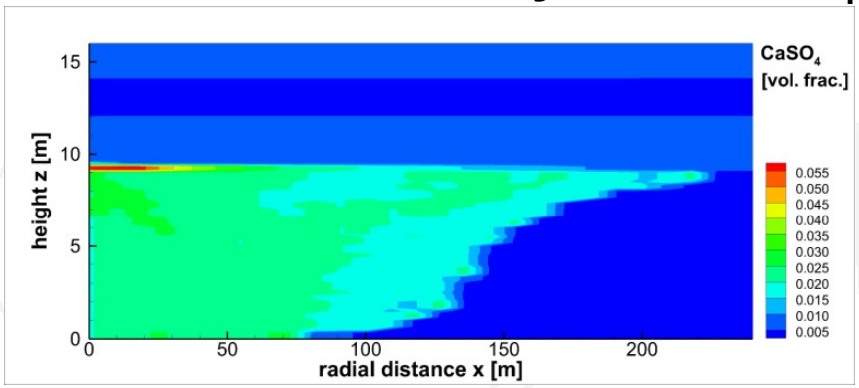
ankerite $CaFe_{0.7}Mg_{0.3}CO_3)_2$



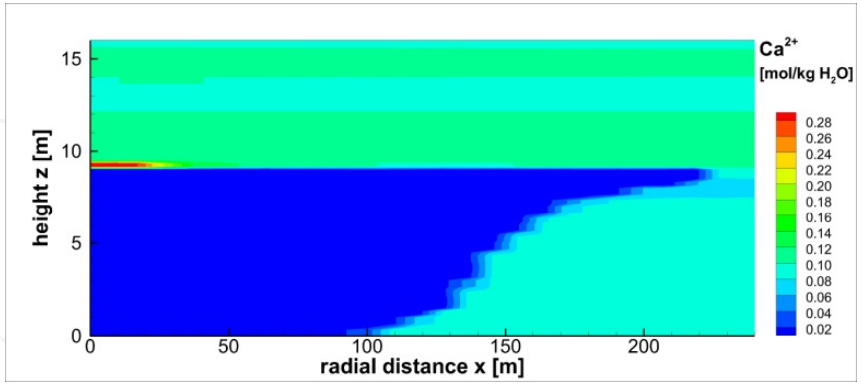
SO_2 (gas)



anhydrite $CaSO_4$



calcium ion Ca^{2+}



solid phases

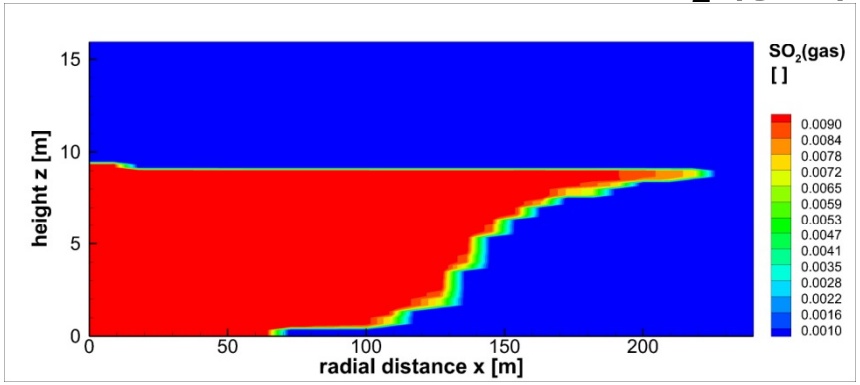
mobile phases

reactive transport

Ca

ankerite $CaFe_{0.7}Mg_{0.3}CO_3)_2$

SO_2 (gas)



anhydrite $CaSO_4$

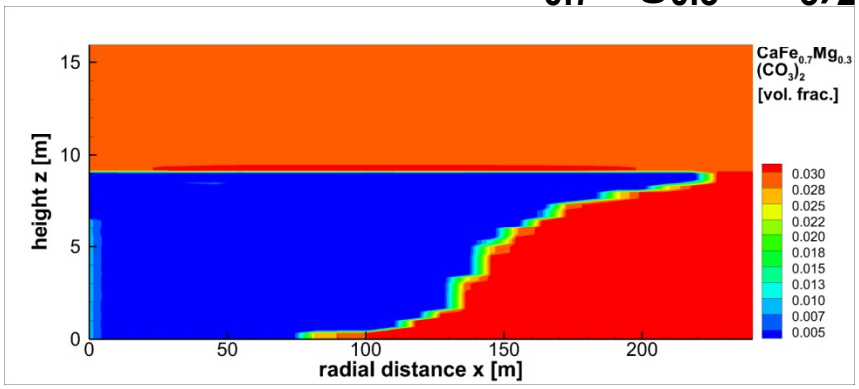
calcium ion Ca^{2+}

SO_2 influences pH value

reactive transport

Ca

ankerite $CaFe_{0.7}Mg_{0.3}CO_3)_2$



SO_2 (gas)

anhydrite $CaSO_4$

calcium ion Ca^{2+}

pH value dissolves ankerite

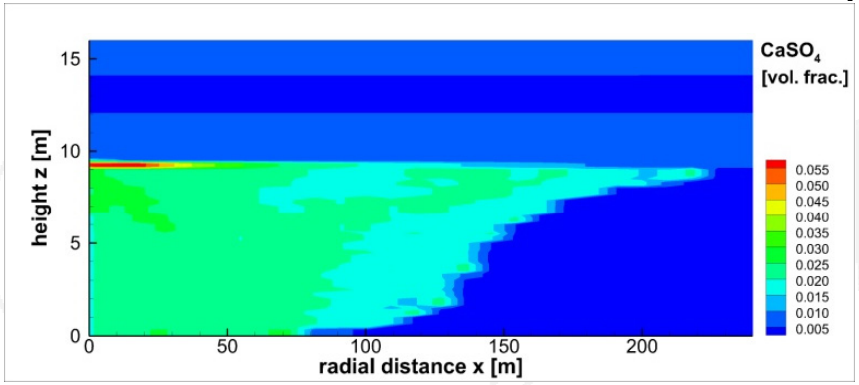
reactive transport

Ca

ankerite $CaFe_{0.7}Mg_{0.3}CO_3)_2$

SO_2 (gas)

anhydrite $CaSO_4$



calcium ion Ca^{2+}

sulfate + calcium leads to anhydrite precipitation

reactive transport

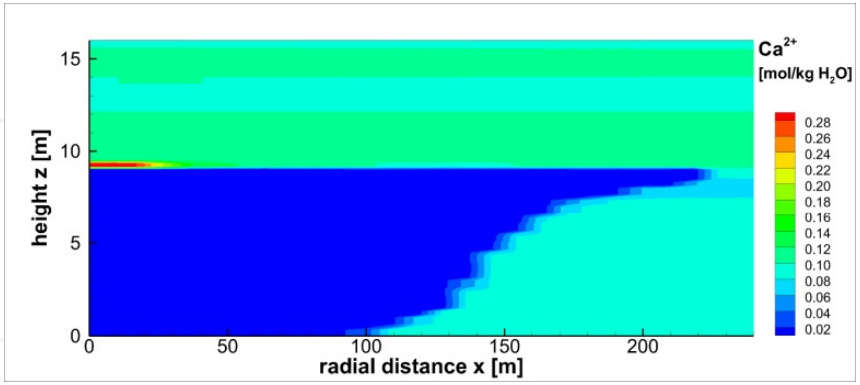
Ca

ankerite $CaFe_{0.7}Mg_{0.3}CO_3)_2$

SO_2 (gas)

anhydrite $CaSO_4$

calcium ion Ca^{2+}

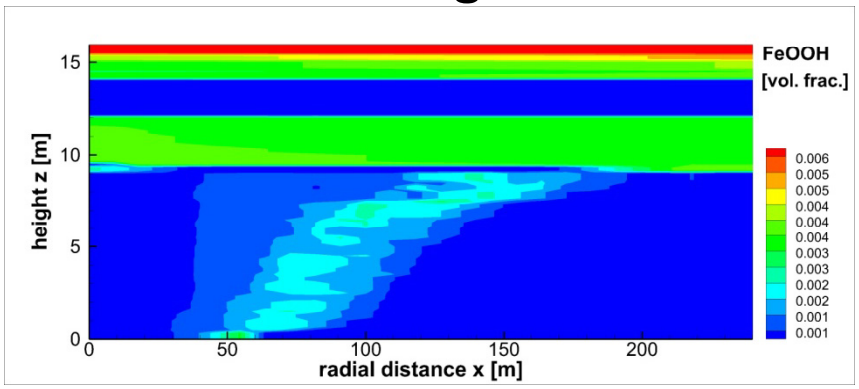


forming anhydrite removes free Ca^{2+}

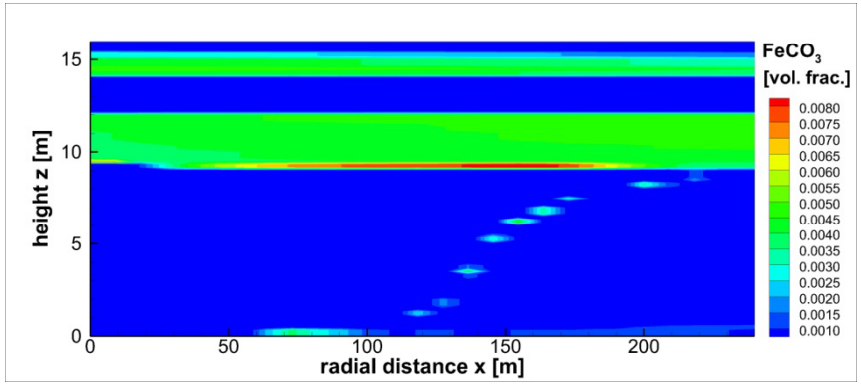
reactive transport

Fe

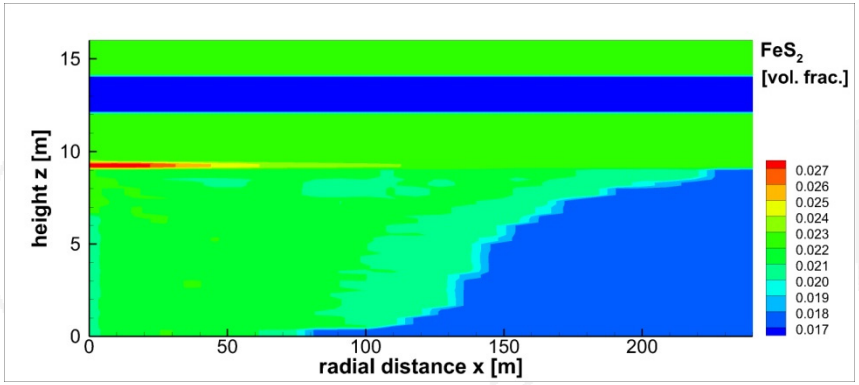
goethite FeOOH



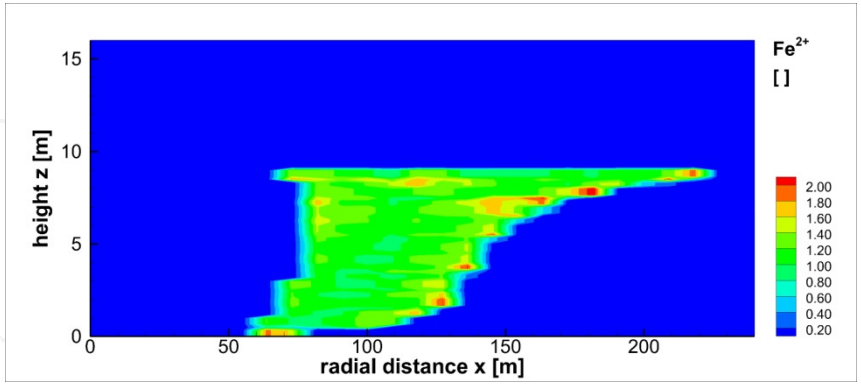
siderite



pyrite FeS_2



iron ion Fe^{2+}



Fe^{2+} is 2nd reacting system

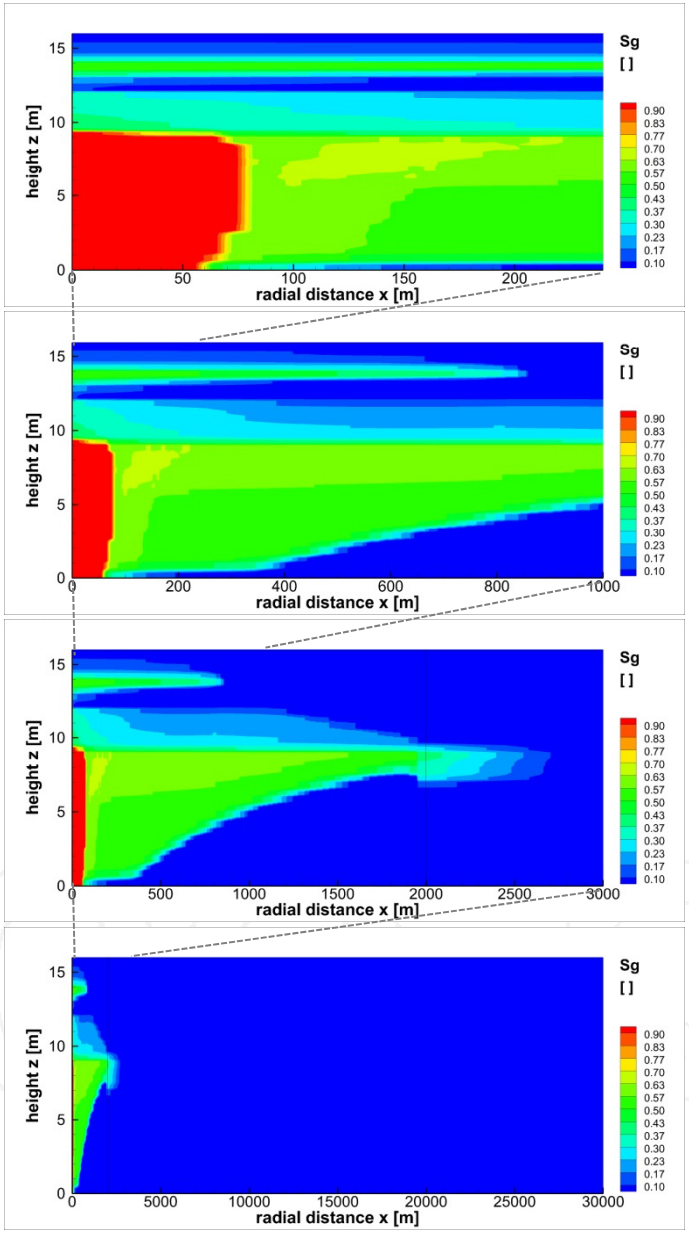
adds complexity

complex interplay

- multiphase, multicomponent transport
- chemical reactivity
- residence time
- flow pattern

reactive transport

reservoir scale



x = 240 m

x = 1000 m

x = 3000 m

x = 30000 m

dry-out zone < 70 m

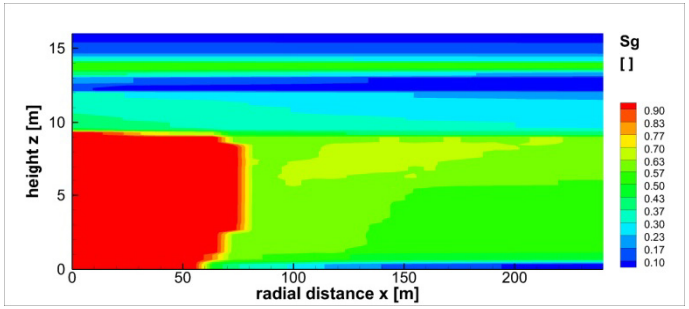
2nd sandstone 800 m

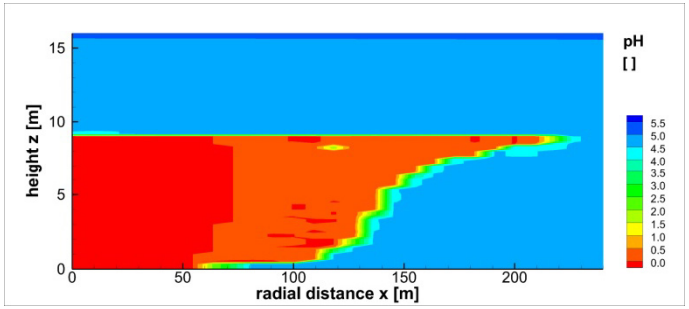
1st sandstone 2500 m

Sg

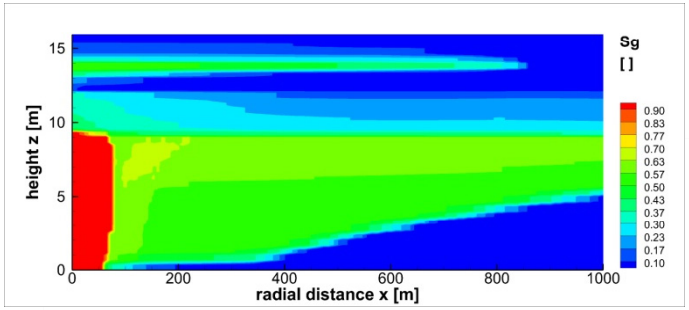
reactive transport

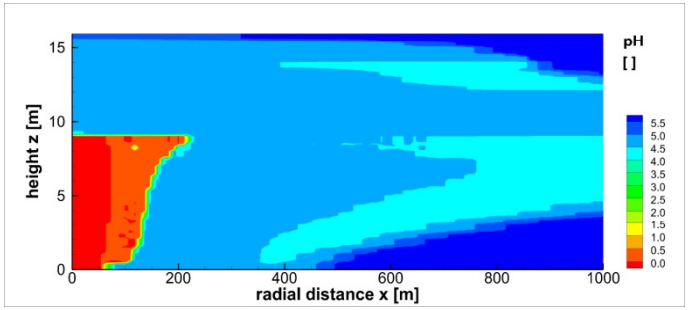
reservoir scale



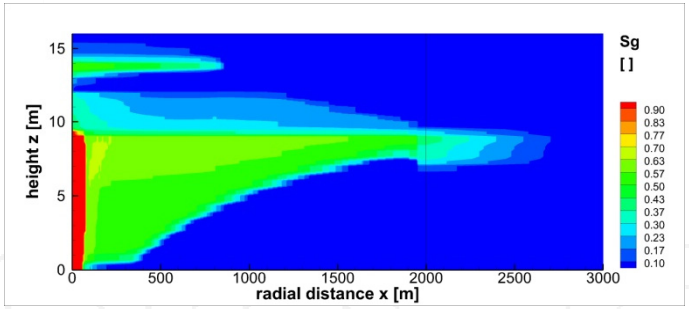


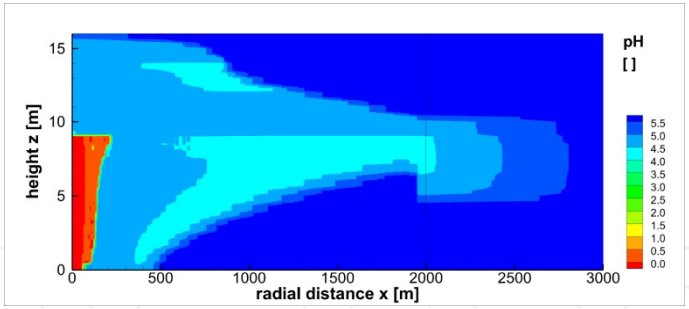
x = 240 m



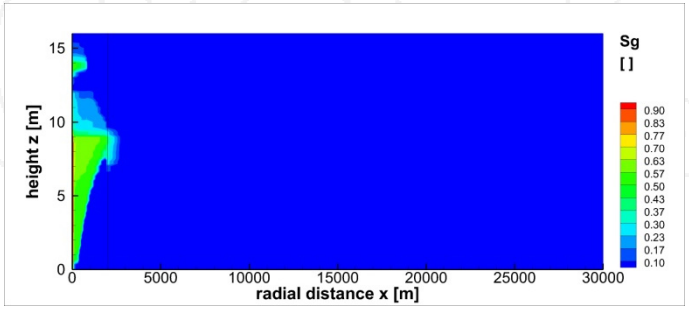


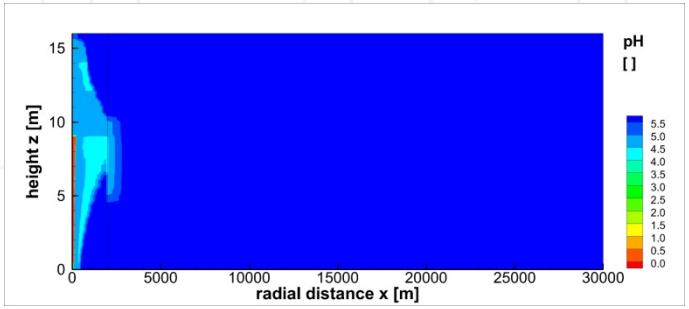
x = 1000 m





x = 3000 m



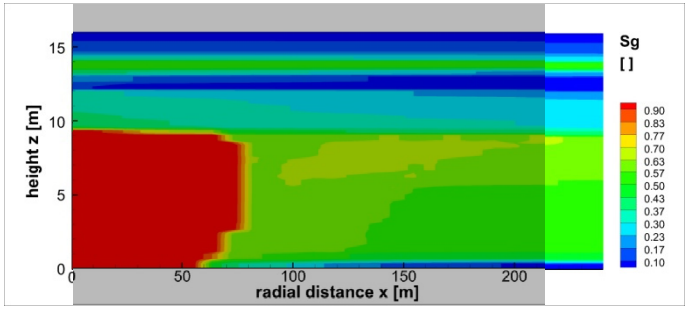


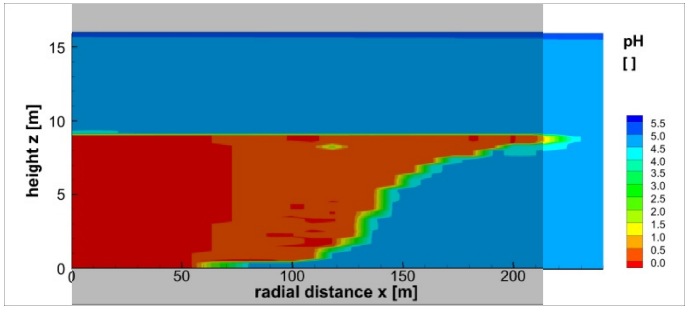
x = 30000 m

Sg **pH**

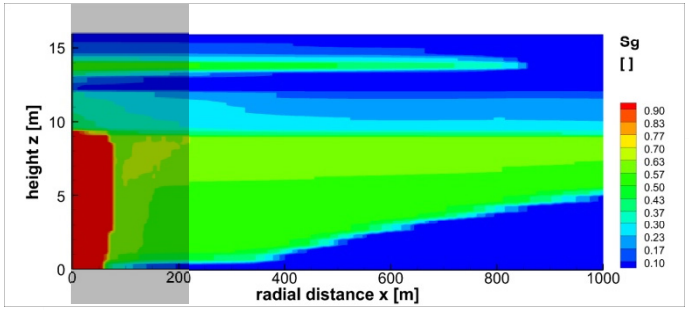
reactive transport

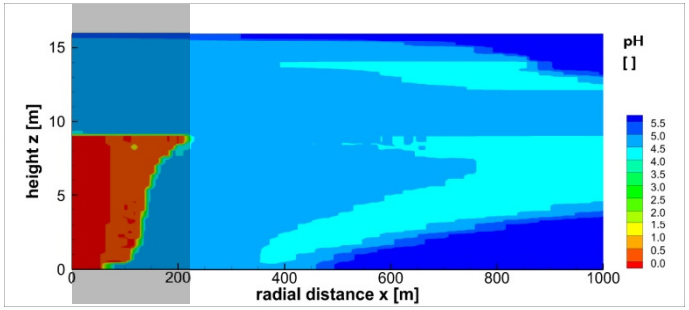
SO_2 influence



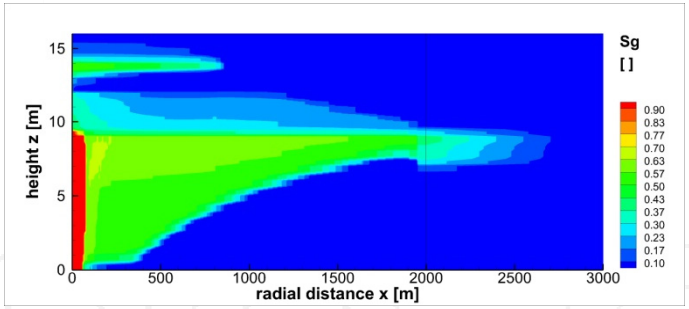


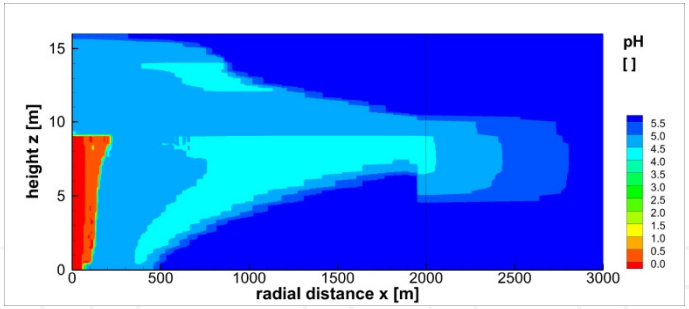
x = 240 m



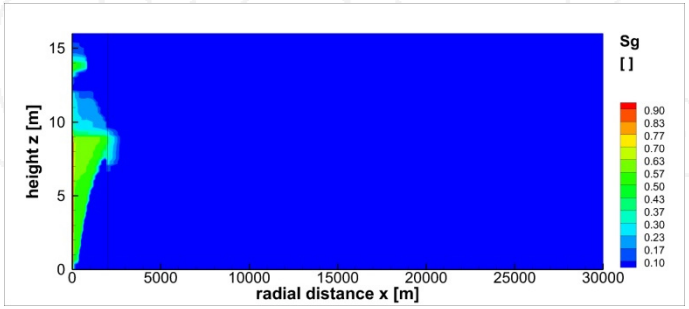


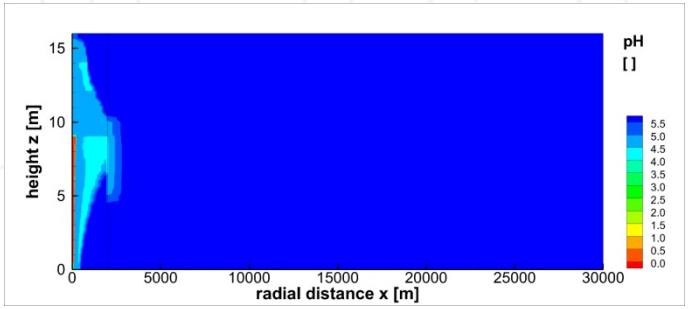
x = 1000 m





x = 3000 m





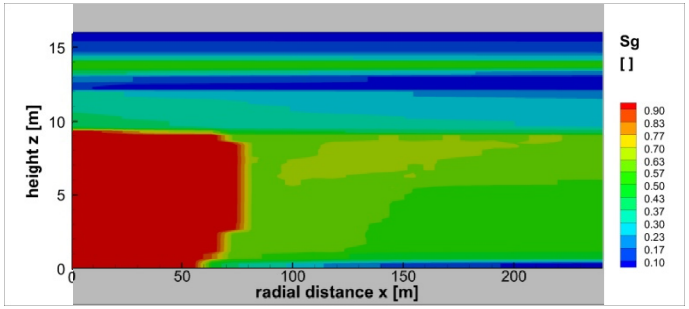
x = 30000 m

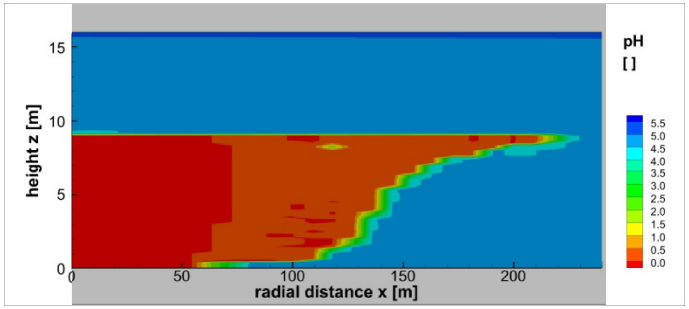
Sg

pH

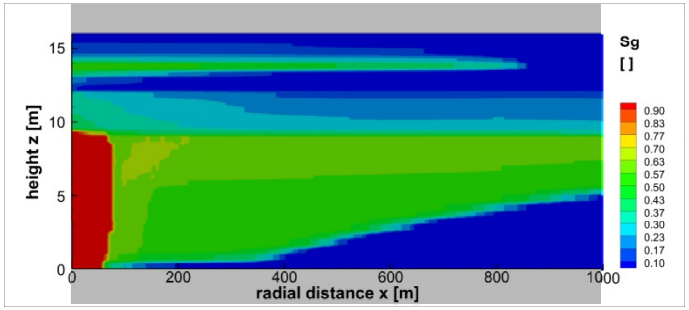
reactive transport

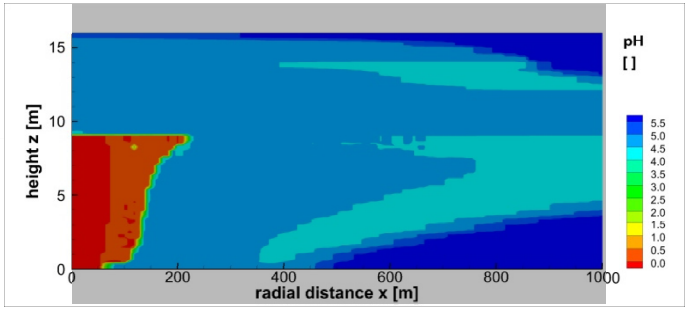
CO_2 influence



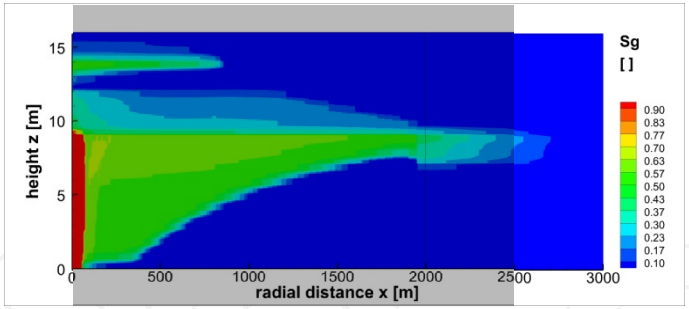


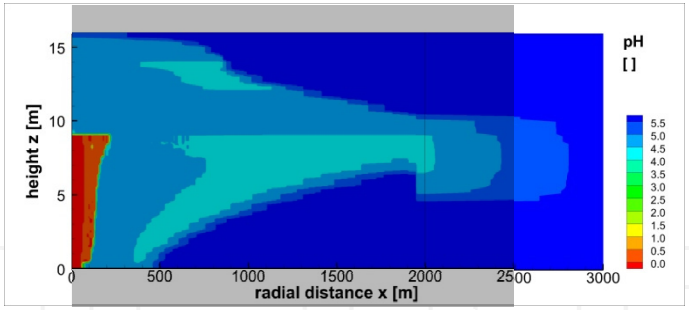
x = 240 m



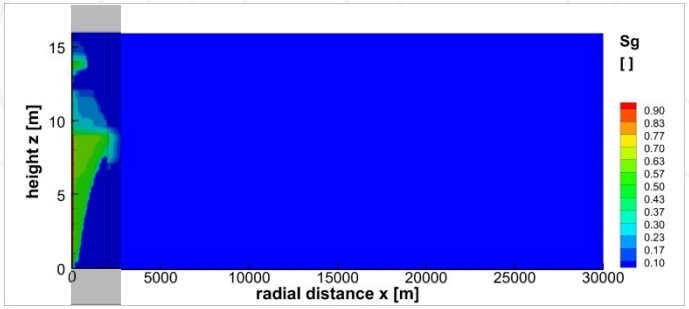


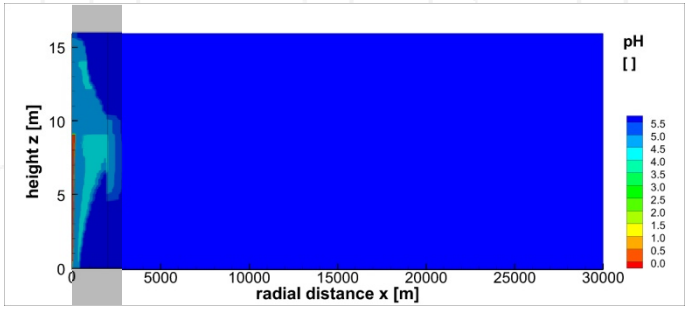
x = 1000 m





x = 3000 m





x = 30000 m

Sg

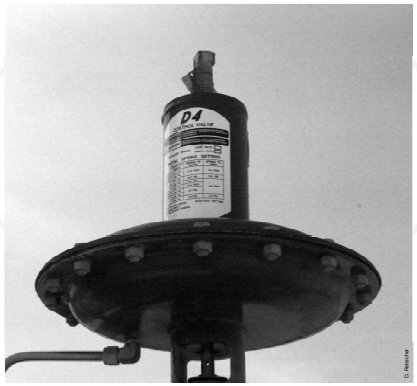
pH

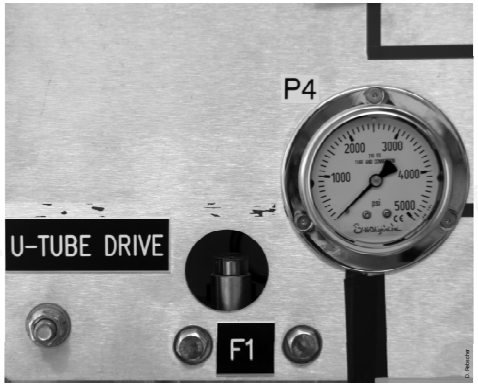
conclusion

main reactivity is determined by initial mineral composition

spatial separation of impact of CO_2 and SO_2

SO_2 200 m, CO_2 2500 m





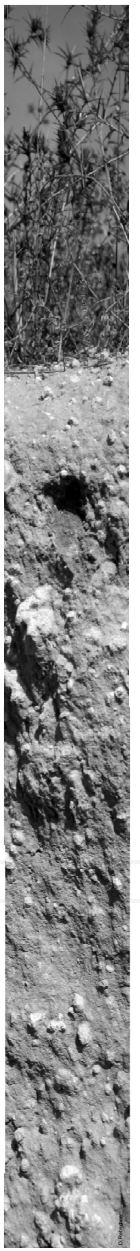
outlook

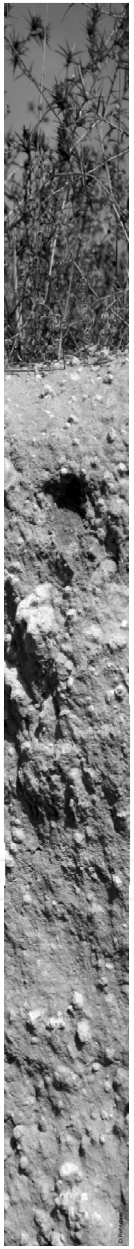
Heletz impure CO_2 injection test
comparison experiment + model

end of CO_2QUEST 6/2016

disclaimer

The research leading to the results described in this presentation has received funding from the European Union 7th Framework Programme FP7-ENERGY-2012-1-2STAGE under grant agreement number 309102.



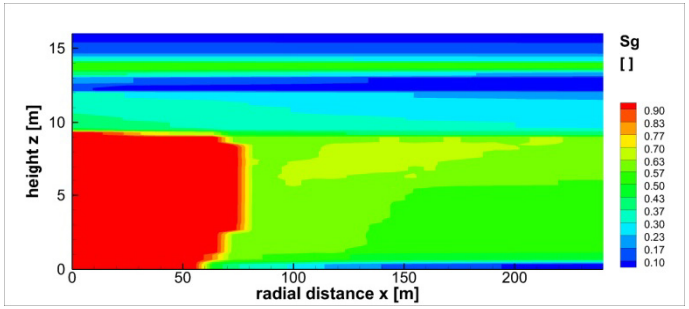


thank you

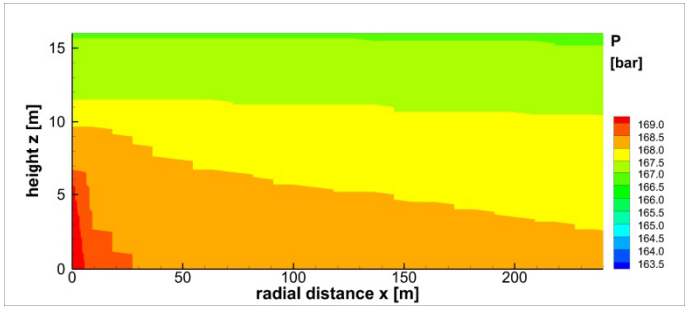
CO_2QUEST

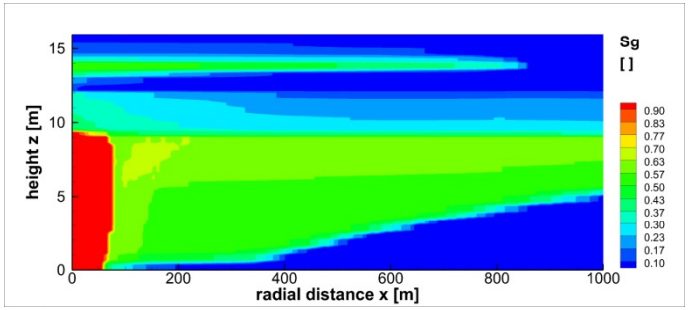
reactive transport

Sg + P

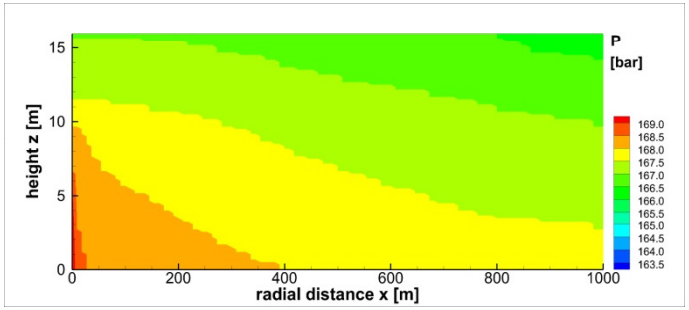


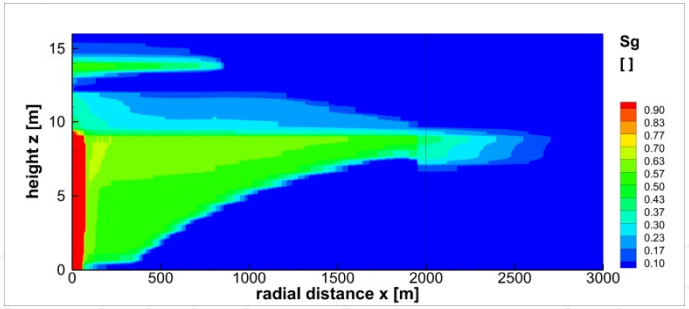
x = 240 m



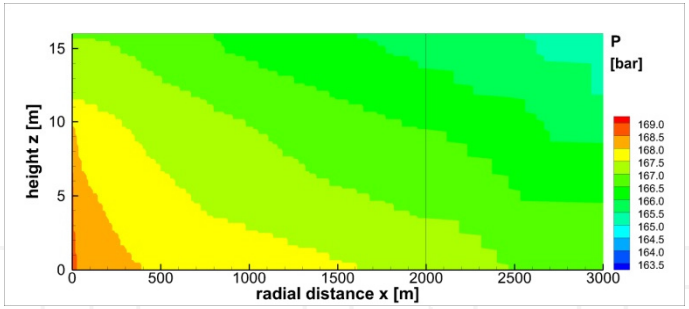


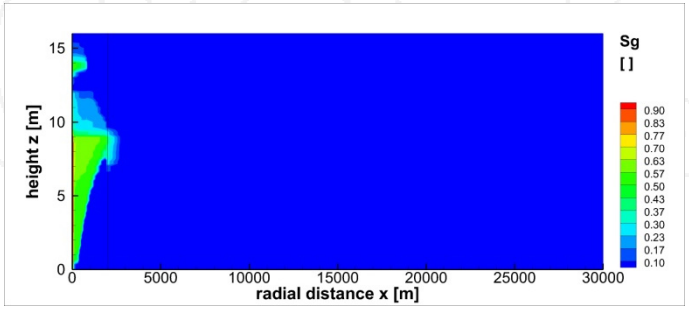
x = 1000 m



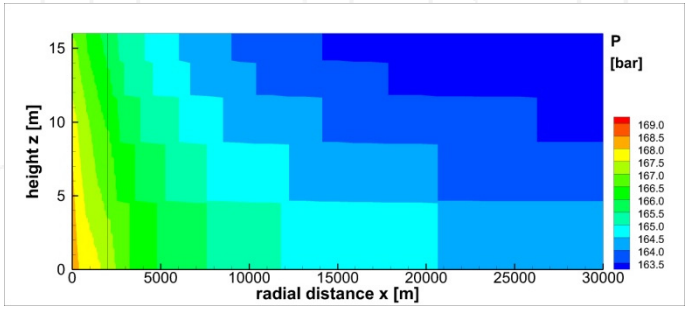


x = 3000 m





x = 30000 m



Sg

P