CO_2QUEST COORAL

* slides + presentation

Comparison of different numerical and modelling approaches for implementing SO_2 as a CO_2 flue gas impurity in geochemical simulations in saline sandstone aquifers

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2nd International Forum on Recent Developments of CCS Implementation
16. – 17. December, Athens, Greece

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COORAL

CO_2 purity for separation and storage

CO_2-Reinheit für die Abscheidung und Lagerung

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CO_2 purity for separation and storage

optimization of the process chain
production – transport – injection – geological storage

what is the optimal composition of the CO_2 stream?

laboratory experiments, numerical modelling

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CO_2QUEST

Impact of the Quality of CO_2 on Storage and Transport

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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**

laboratory + field experiments, numerical modelling

CO_2QUEST

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

laboratory + field experiments, **numerical modelling**

two comparisons

I Heletz sandstone, Israel
Rotliegend sandstone, Germany
Bunter sandstone, Germany

II basic geochemical batch simulations – PHREEQC
reactive transport simulations – TOUGHREACT
time/spatial info

same measured and calculated data set of Heletz as used before
i.e. mineral composition, in situ pT, formation water chemistry

initial parameter

base model	porosity [%]	p [MPa]	T [°C]	S [ ]	brine	quartz [%]	clay minerals [%]	feldspars [%]	carbonates [%]	others [%]
Bunter	20	15.0	55	0.231	NaCl	63	6	16	9	6
Rotliegend	10	32.0	90	0.250	NaCl	63	9	11	10	7
Heletz	20	14.7	66	0.055	NaCl	69	9	16	4	2

batch simulation PHREEQC V3

constant volume of the impure CO_2 stream
1 % SO_2

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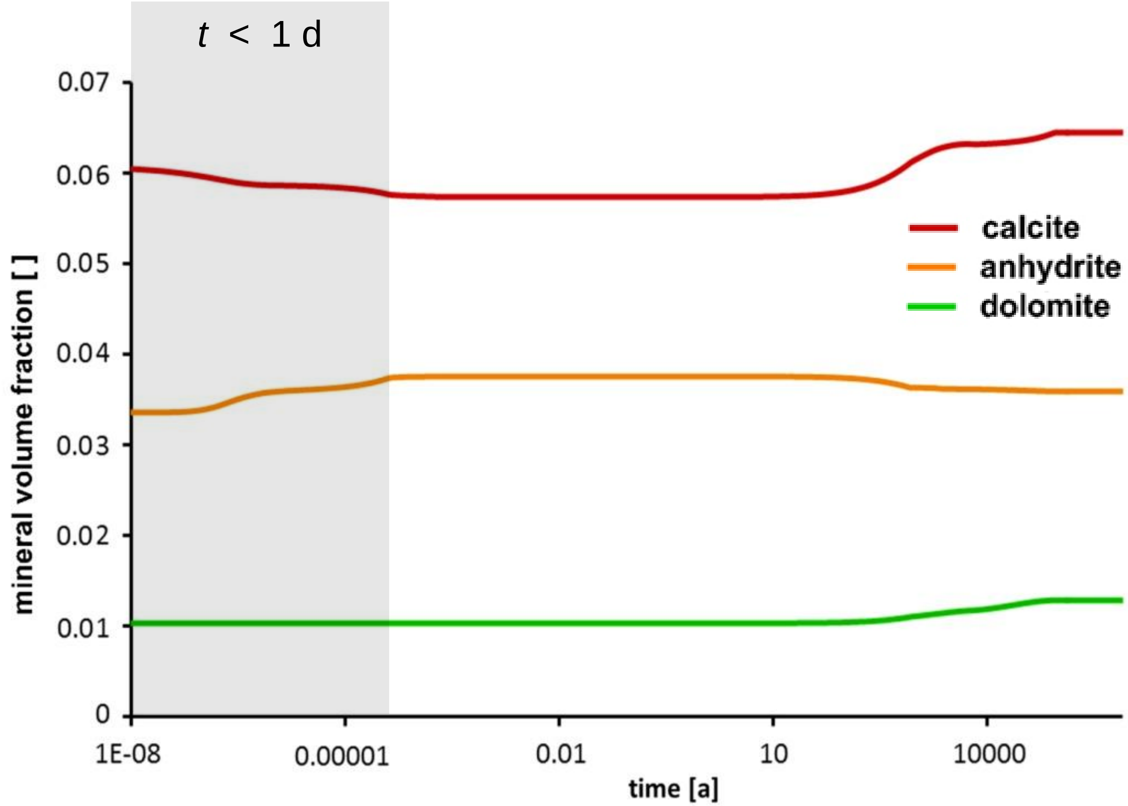
batch simulation Bunter

Ca^{2+}

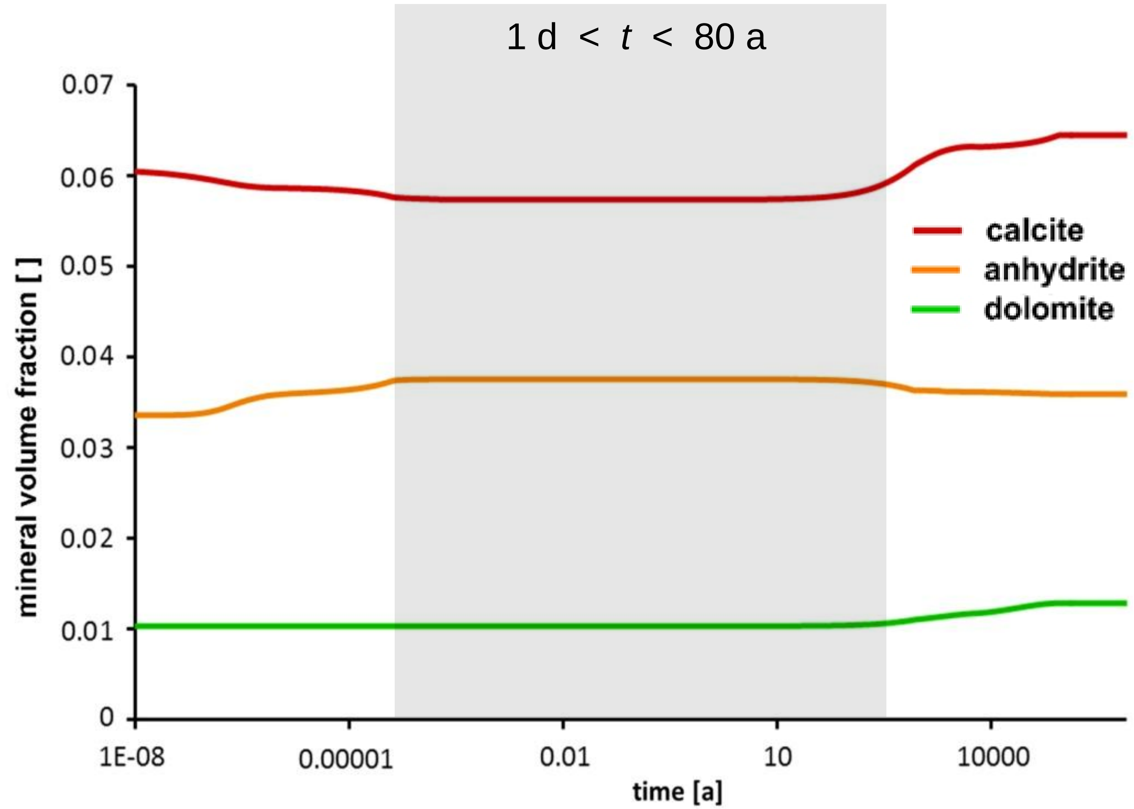


establish equilibrium

calcite $CaCO_3$	**dissolves**
anhydrite $CaSO_4$	**precipitates**
dolomite $CaMg(CO_3)_2$ ($CaCO_3 \cdot MgCO_3$))	**stable**

batch simulation Bunter

Ca^{2+}

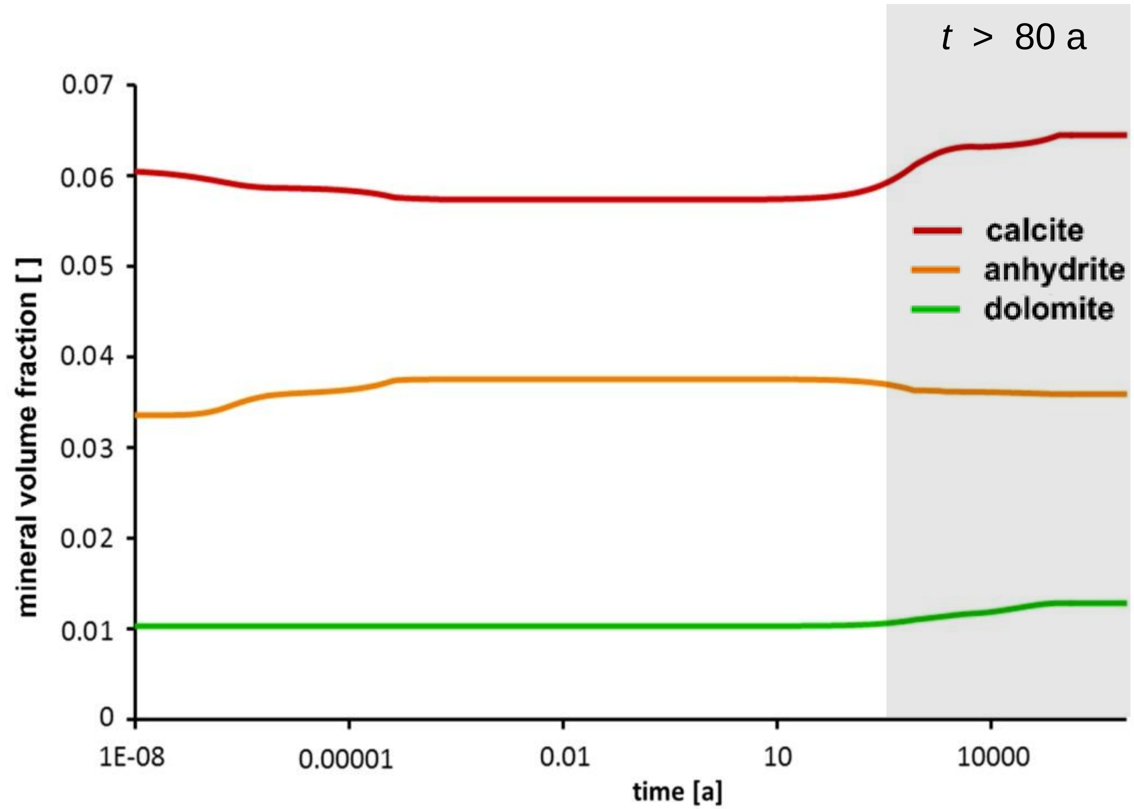


quasi stationary equilibrium of fast reacting minerals

calcite $CaCO_3$	**constant**
anhydrite $CaSO_4$	**constant**
dolomite $CaMg(CO_3)_2$ ($CaCO_3 \cdot MgCO_3$))	**constant**

batch simulation Bunter

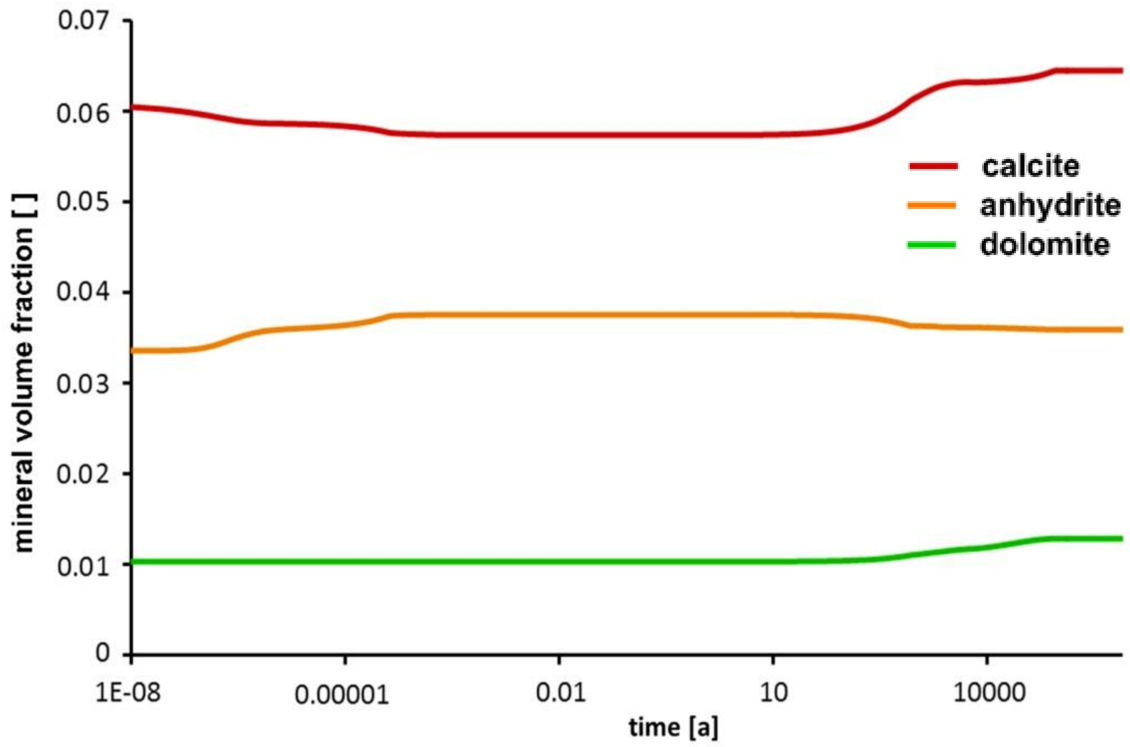
Ca^{2+}



calcium precipitation from slow reacting feldspars

calcite $CaCO_3$	**precipitates**
anhydrite $CaSO_4$	**dissolves**
dolomite $CaMg(CO_3)_2$ ($CaCO_3 \cdot MgCO_3$))	**precipitates**

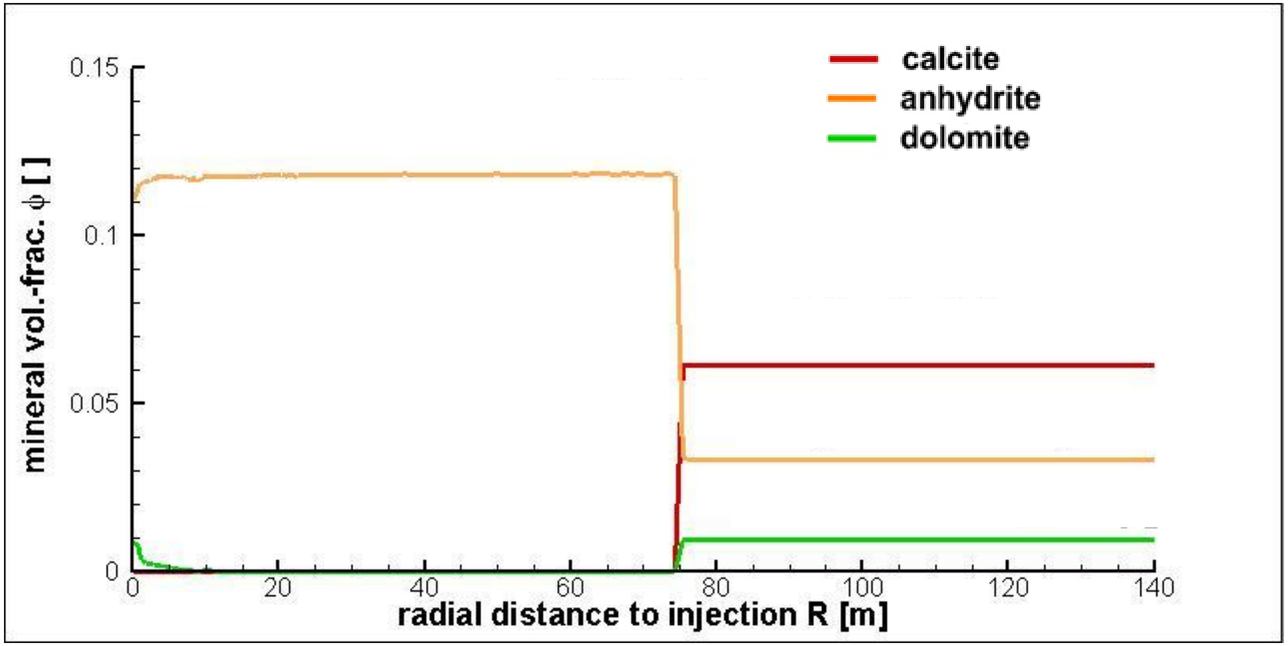
batch simulation Bunter



short-term establishing equilibrium of fast reacting minerals

long-term transformation of feldspars to carbonates

reactive transport Bunter minerals

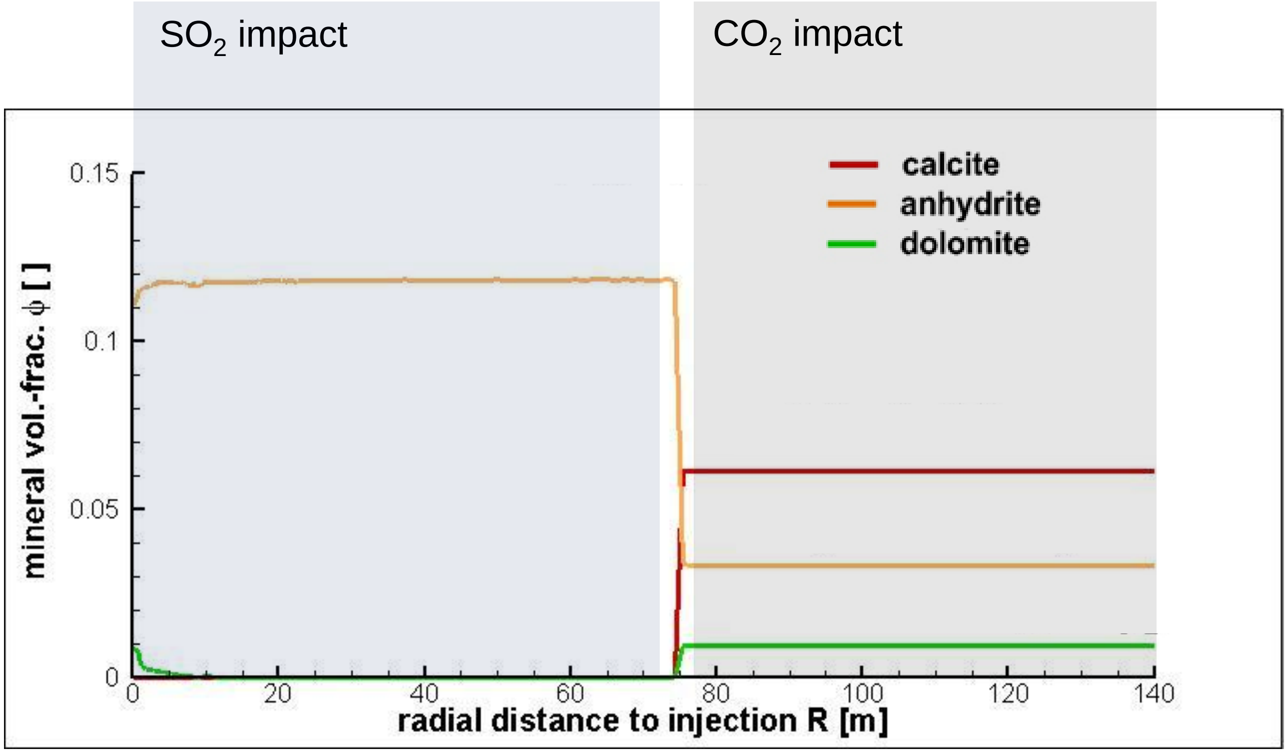


1D radial reactive transport spatial profile

TOUGHREACT OMP-3.0 ECO2N
impure CO_2 stream 9 kg/s, 1 % SO_2

reactive transport Bunter

minerals



range of SO_2 impact < 75 m
CO_2 impact > 75 m

reactive transport parameters

base model	porosity [%]	p [MPa]	T [°C]	S [ ]	brine	quartz [%]	clay minerals [%]	feldspars [%]	carbonates [%]	others [%]
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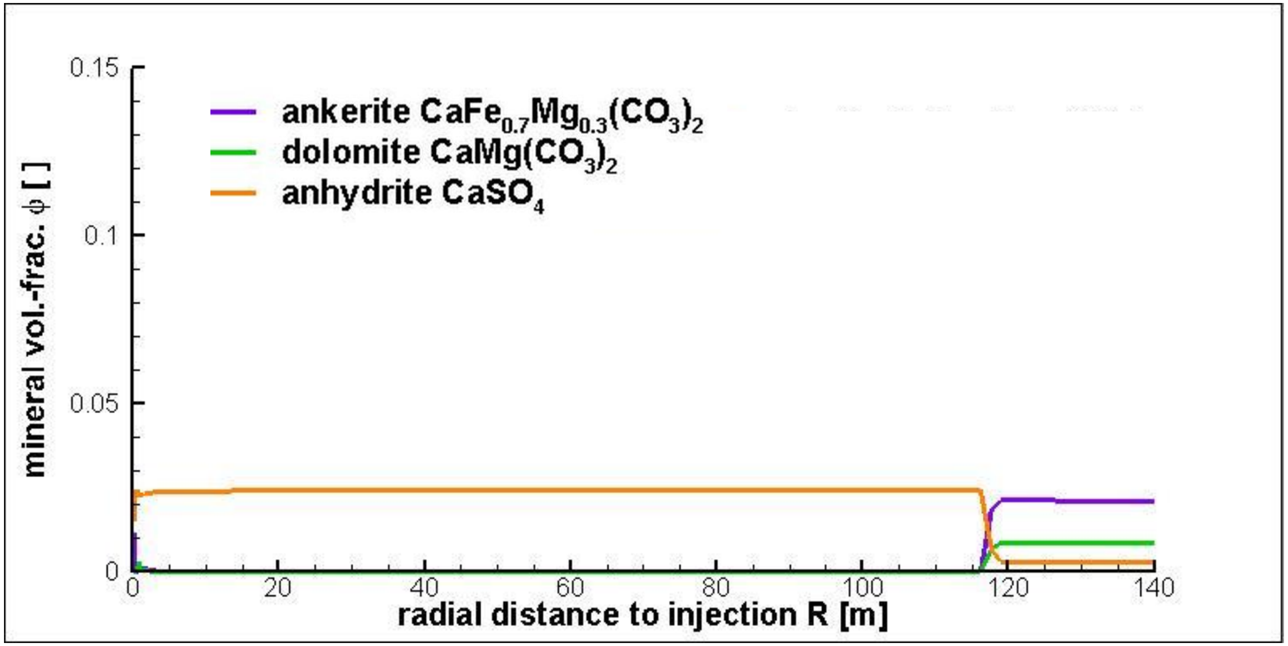
reactive transport Heletz

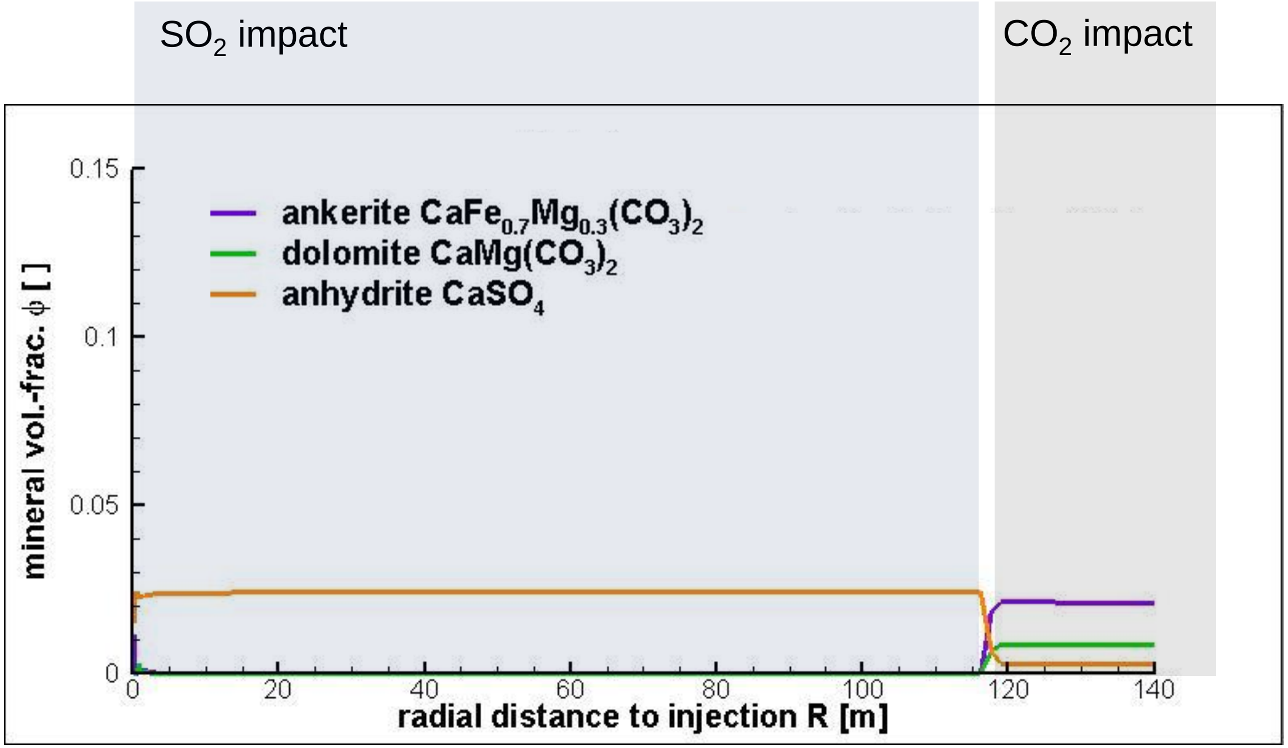
minerals



1D radial reactive transport spatial profile

reactive transport Heletz

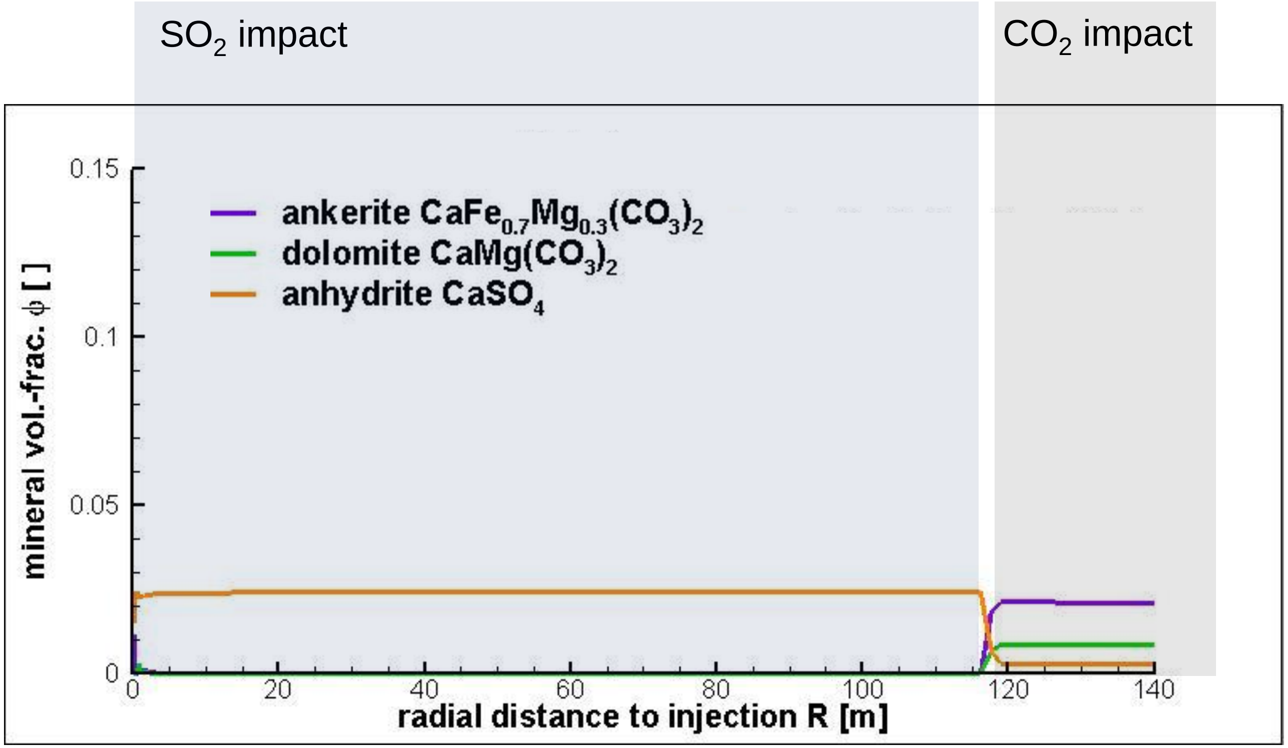
minerals



range of SO_2 impact < 115 m
CO_2 impact > 115 m

reactive transport Heletz

minerals



	Heletz	Bunter
range of SO_2 impact	< 115 m	< 75 m
CO_2 impact	> 115 m	< 75 m

Bunter

high carbonates, i.e. calcite $CaCO_3$ and dolomite $CaMg(CO_3)_2$
almost complete dissolution

precipitation as anhydrite $CaSO_4$

	Heletz	Bunter
range of SO_2 impact	< 115 m	< 75 m
CO_2 impact	> 115 m	< 75 m

Bunter

high carbonates, i.e. calcite $CaCO_3$ and dolomite $CaMg(CO_3)_2$
almost complete dissolution

precipitation as anhydrite $CaSO_4$

molar volume	$CaCO_3$	37 cm^3/mol
	$CaMg(CO_3)_2$	64 cm^3/mol
	$CaSO_4$	46 cm^3/mol

decrease in porosity

Bunter

high carbonates, i.e. calcite $CaCO_3$ and dolomite $CaMg(CO_3)_2$
almost complete dissolution

after 10 years, injected SO_2 used up within 75 m

Heletz

less and different carbonates,

more rock volume needed to use SO_2

larger dry out zone

after 10 years, injected SO_2 used up within 115 m

Heletz

less and different carbonates,
i.e. ankerite $CaFe_{0.7}Mg_{0.3}(CO_3)_2$ and dolomite $CaMg(CO_3)_2$
almost complete dissolution

less Ca^{2+} in ankerite than in calcite $CaCO_3$

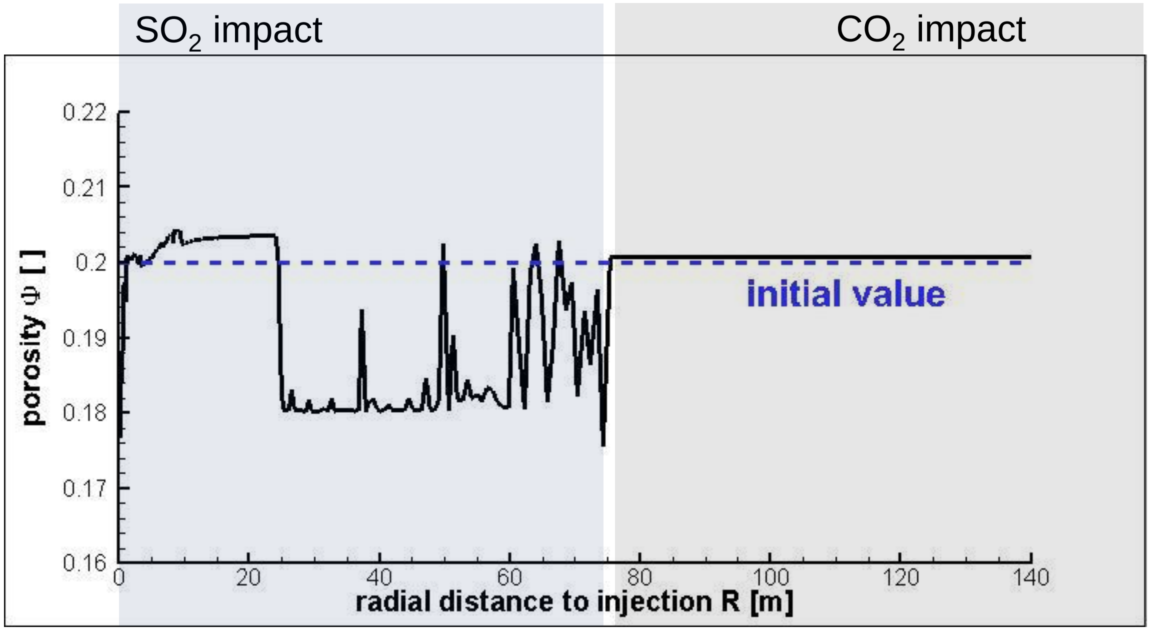
less precipitation as anhydrite $CaSO_4$

increase in porosity

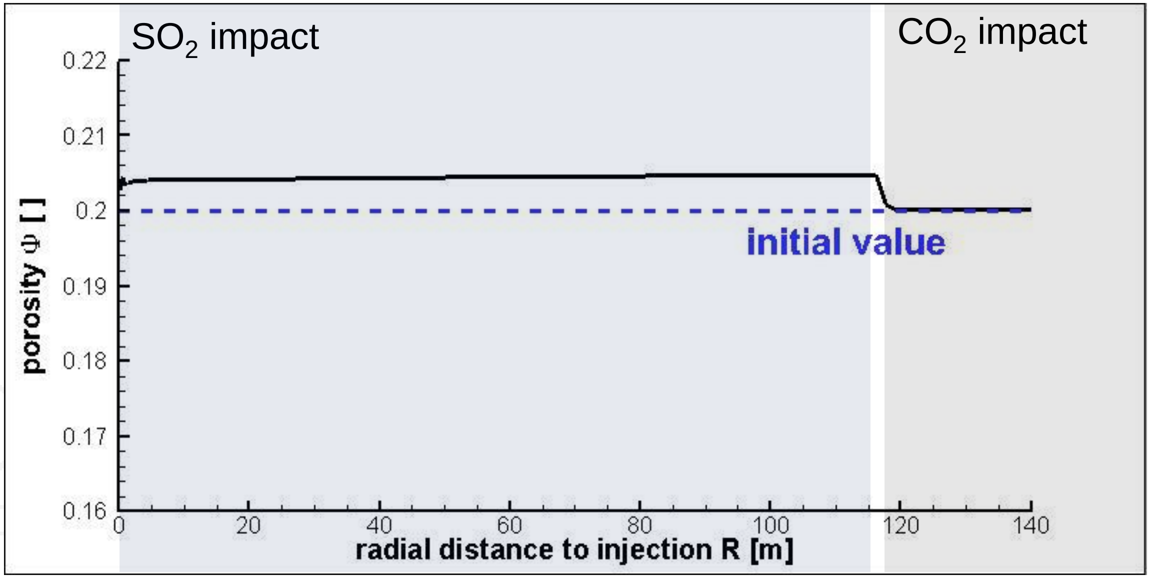
reactive transport

porosty

Bunter



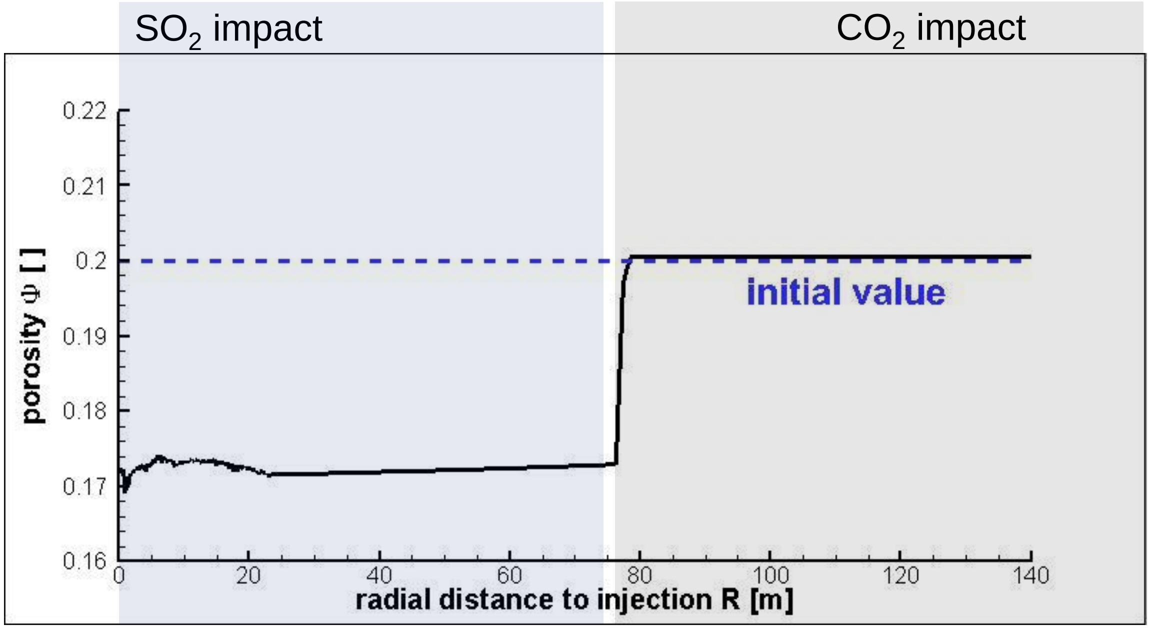
Heletz



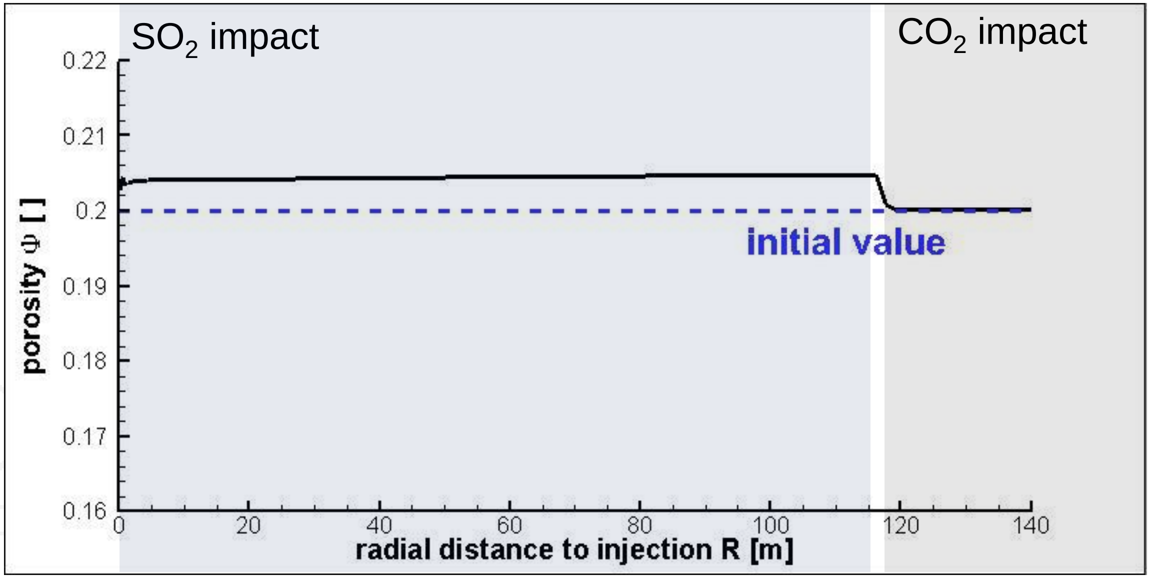
reactive transport porosty

Bunter

was albite $NaAlSi_3O_8$ now oligoclase $(Ca,Na)(Al,Si)_4O_8$



Heletz



conclusion

PHREEQC and TOUGHREACT, complements

preferential dissoluton of SO_2 compared to CO_2
together with
high reactivity with carbonates
→ spatial separation

amount and species of carbonates
→ determine porosity

other minerals play minor part

outlook

end of CO_2QUEST 6/2016

3rd sandstone Rotliegend

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 and from the German Federal Ministry for Economic Affairs and Energy.

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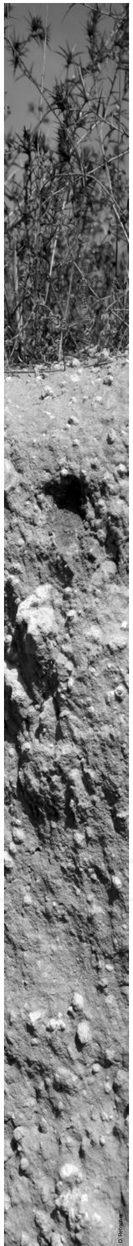

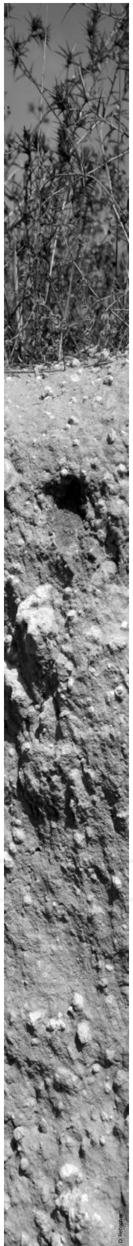

thank you