VISUALIZATION OF GEOCHEMICAL MODELING RESULTS BY R

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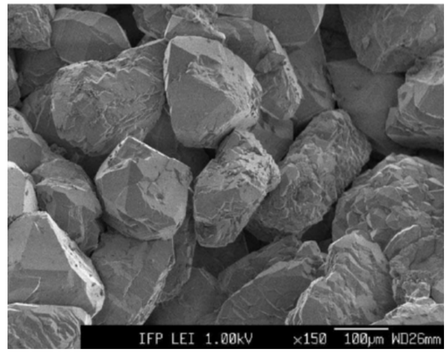
2016 SATRDAY BUDAPEST

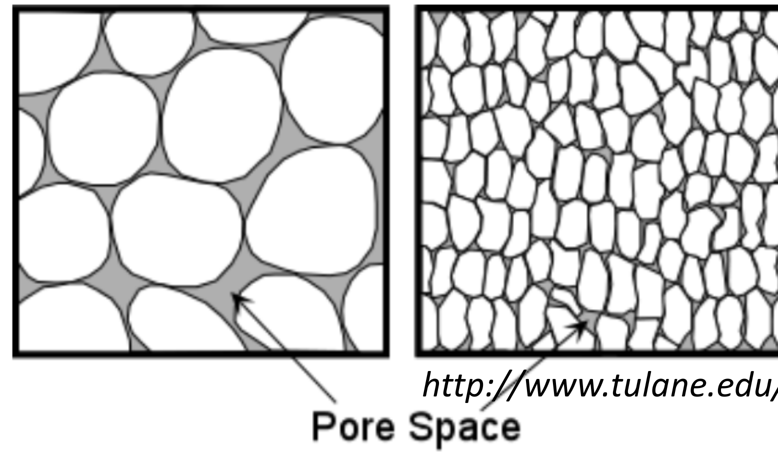
MFGI
MAGYAR FÖLDTANI ÉS GEOFIZIKAI INTÉZET

What is geochemical modeling?

Rock: naturally occurring solid aggregate of minerals



Montaron & Han 2009



http://www.tulane.edu/

Modeling of chemical reactions between rock and porewater (if I keep it simple)

Thermodynamic vs. kinetic geochemical models

Final, equilibrium state — Considers the speed of reactions

Reactive transport models: geochemical reactions while fluid flows through the pore space

Examples for application:

- Migration of contaminants in the subsurface
- Improving estimates of elemental and nutrient fluxes
- Magma transport in the Earth
- Oil and gas exploration and production
- Building material degradation underground
- CO_2 geological storage (CCS)

Steefel et al. 2005

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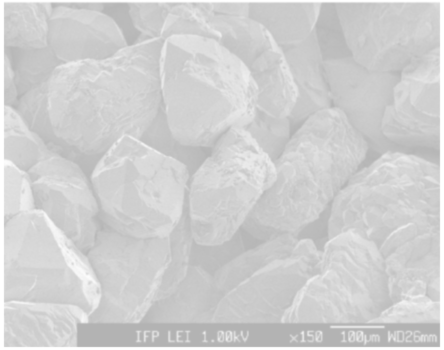

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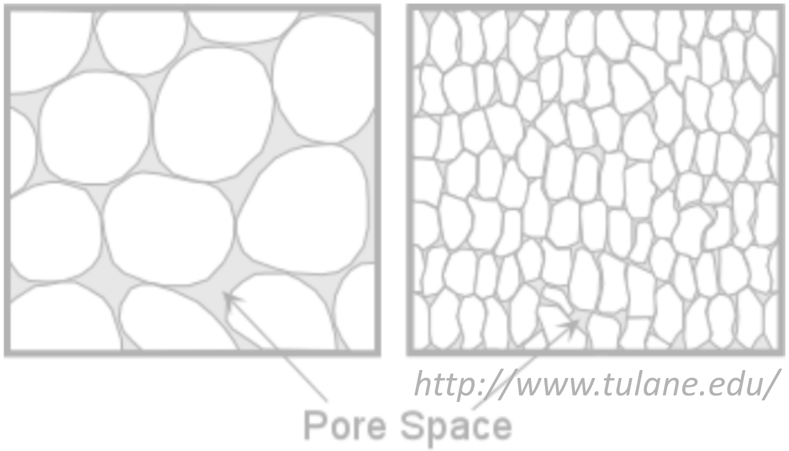

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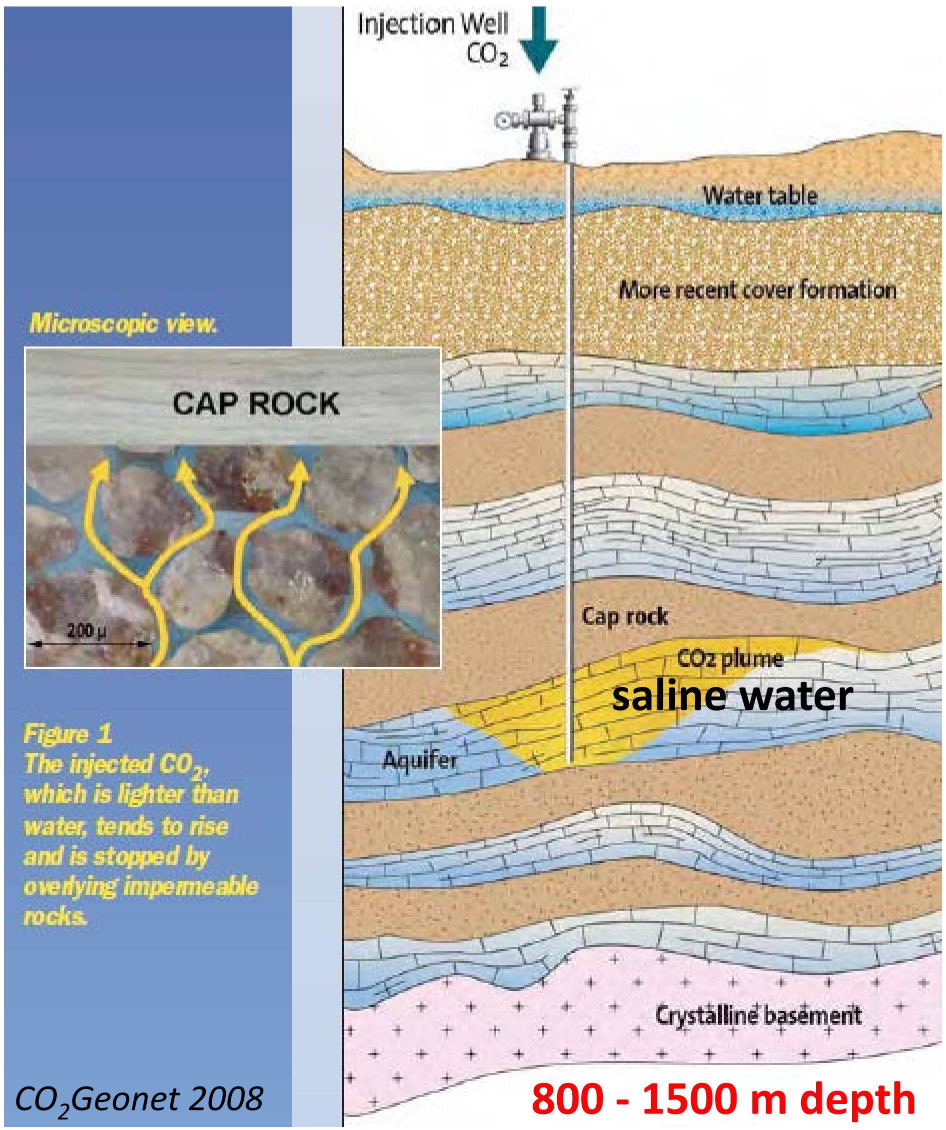
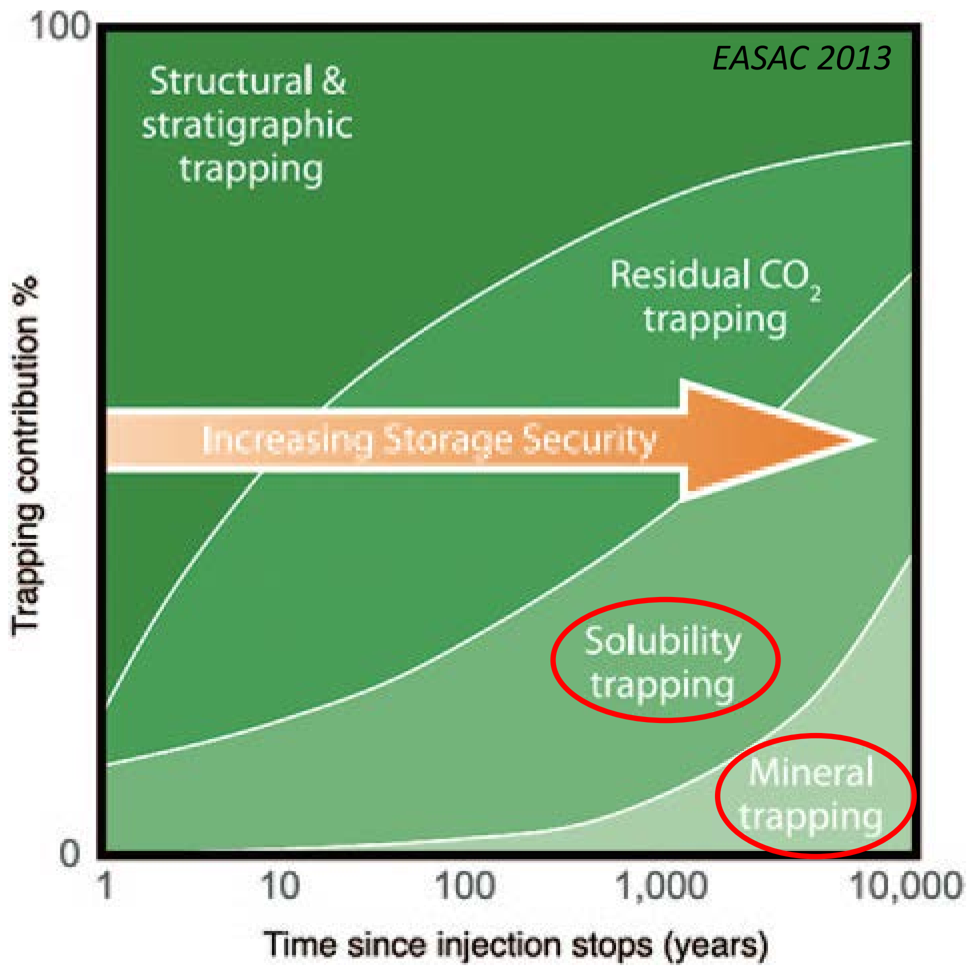
CO_2 geological storage

Power plant → CO_2 capture





USGS
science for a changing world

PHREEQC (Version 3)--A Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations

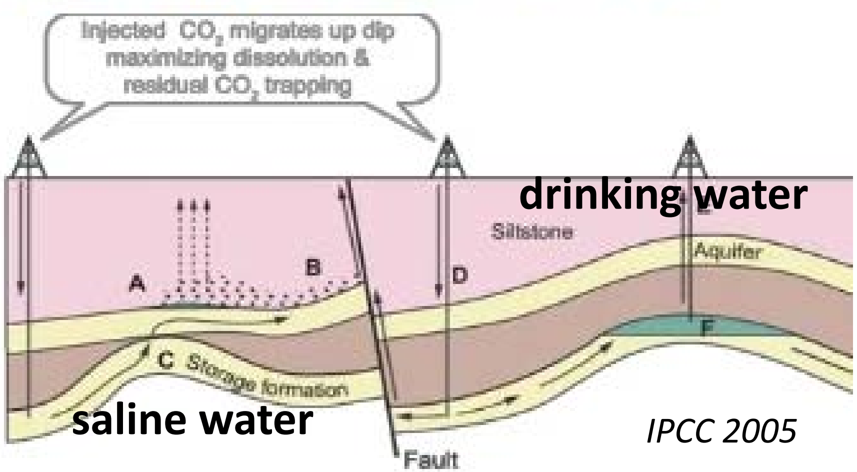
Thermodynamic mixing models

One of the disaster/**worst-case scenarios** at a potential CO_2 geological storage site:

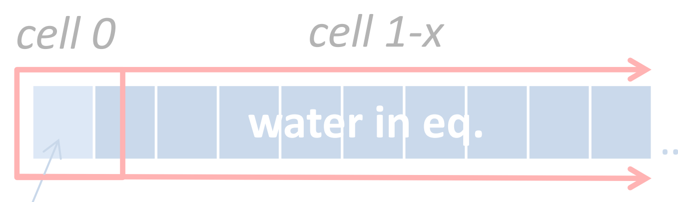
CO_2 leaks into shallower **drinking water aquifer**

What happens at different leakage levels?

Leakage Scenarios



1D reactive transport models with kinetic geochemical reactions



CO_2 saturated water in eq.

Effect of injected CO_2 on storage rock:

- What minerals dissolve?
- How it changes the solution composition?
- What minerals precipitate?
- Potentially, how it changes the porosity and physical properties of the rock?

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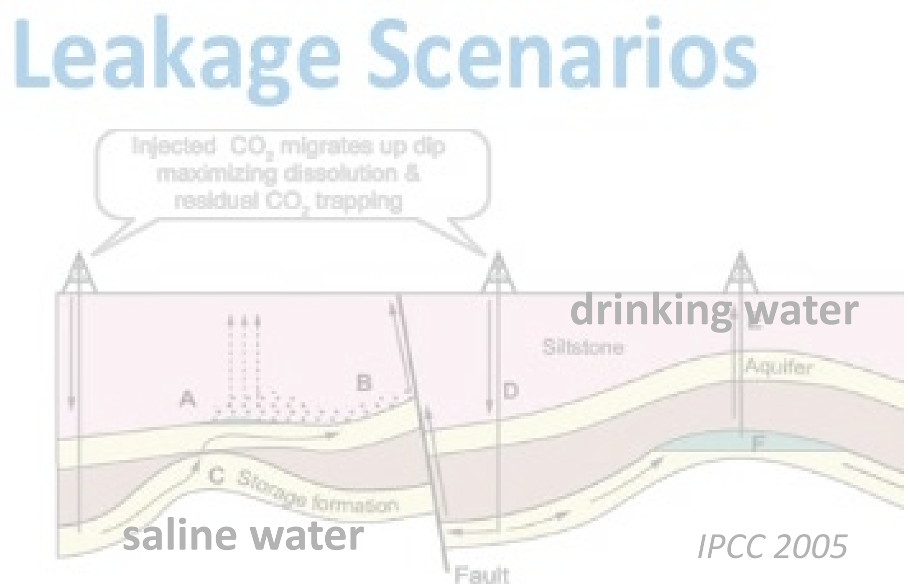

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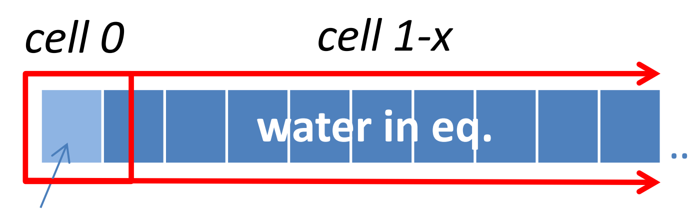

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Why R is used for figure production?

Personal choice…

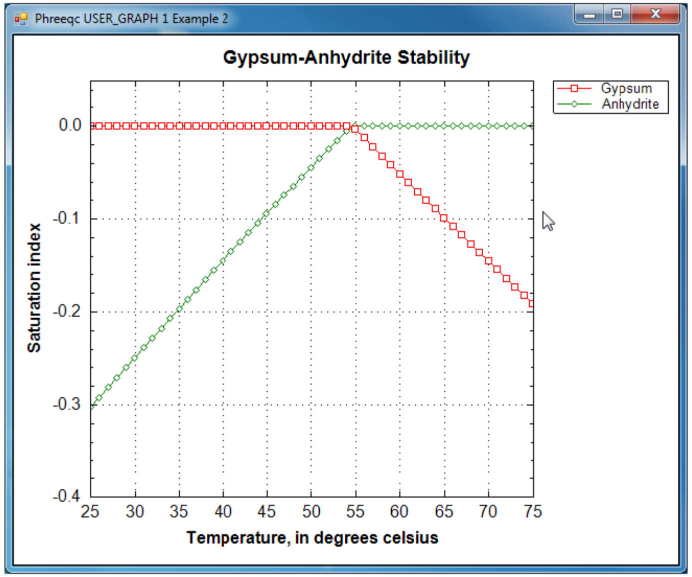
Microsoft Excel???

PHREEQC USER_GRAPH??? →

Flexibility is low

No possibility for making animations

Saving the figures is difficult



Applied R packages

dplyr reshape2 ggplot2 animation

Thermodynamic mixing

CO_2 leaks into shallower **drinking water aquifer**

dplyr select | **reshape2** melt | **ggplot2** ggplot

```
min_toPlot<-melt(min, id=c('step'))
names(min_toPlot)[2]<-"változó"
plotMIN<-ggplot(min_toPlot)
plotMIN<-plotMIN+geom_line(aes(x = step, y = value, colour = változó,
                           linetype = változó))
```

	step	Albite	Calcite	Chlorite(14A)	Dolomite	Goethite	K-feldspar	Kaolinite	Quartz
1	1	5.5549	3.1017	1.8123	0.82822	4.6454	4.2774	6.3562	149.76
2	2	5.5549	3.1007	1.8121	0.82922	4.6454	4.2774	6.3564	149.76
3	3	5.5549	3.0997	1.8119	0.83022	4.6454	4.2774	6.3566	149.76
4	4	5.5549	3.0987	1.8117	0.83122	4.6454	4.2774	6.3568	149.76
5	5	5.5549	3.0977	1.8115	0.83222	4.6454	4.2774	6.3570	149.76
6	6	5.5549	3.0967	1.8113	0.83322	4.6454	4.2774	6.3572	149.76
7	7	5.5549	3.0957	1.8111	0.83422	4.6454	4.2774	6.3574	149.76
8	8	5.5549	3.0947	1.8109	0.83522	4.6454	4.2774	6.3576	149.76
9	9	5.5549	3.0937	1.8107	0.83621	4.6454	4.2774	6.3578	149.76
10	10	5.5549	3.0927	1.8105	0.83721	4.6454	4.2774	6.3580	149.76
11	11	5.5549	3.0917	1.8103	0.83821	4.6454	4.2774	6.3582	149.76
12	12	5.5549	3.0907	1.8101	0.83921	4.6454	4.2774	6.3584	149.76
13	13	5.5549	3.0897	1.8099	0.84021	4.6454	4.2774	6.3586	149.76
14	14	5.5549	3.0887	1.8097	0.84121	4.6454	4.2774	6.3588	149.76
15	15	5.5549	3.0877	1.8095	0.84221	4.6454	4.2774	6.3590	149.76
16	16	5.5549	3.0867	1.8093	0.84321	4.6454	4.2774	6.3592	149.76
17	17	5.5549	3.0857	1.8091	0.84421	4.6454	4.2774	6.3594	149.76
18	18	5.5549	3.0847	1.8089	0.84521	4.6454	4.2774	6.3596	149.76
19	19	5.5549	3.0837	1.8087	0.84621	4.6454	4.2774	6.3598	149.76

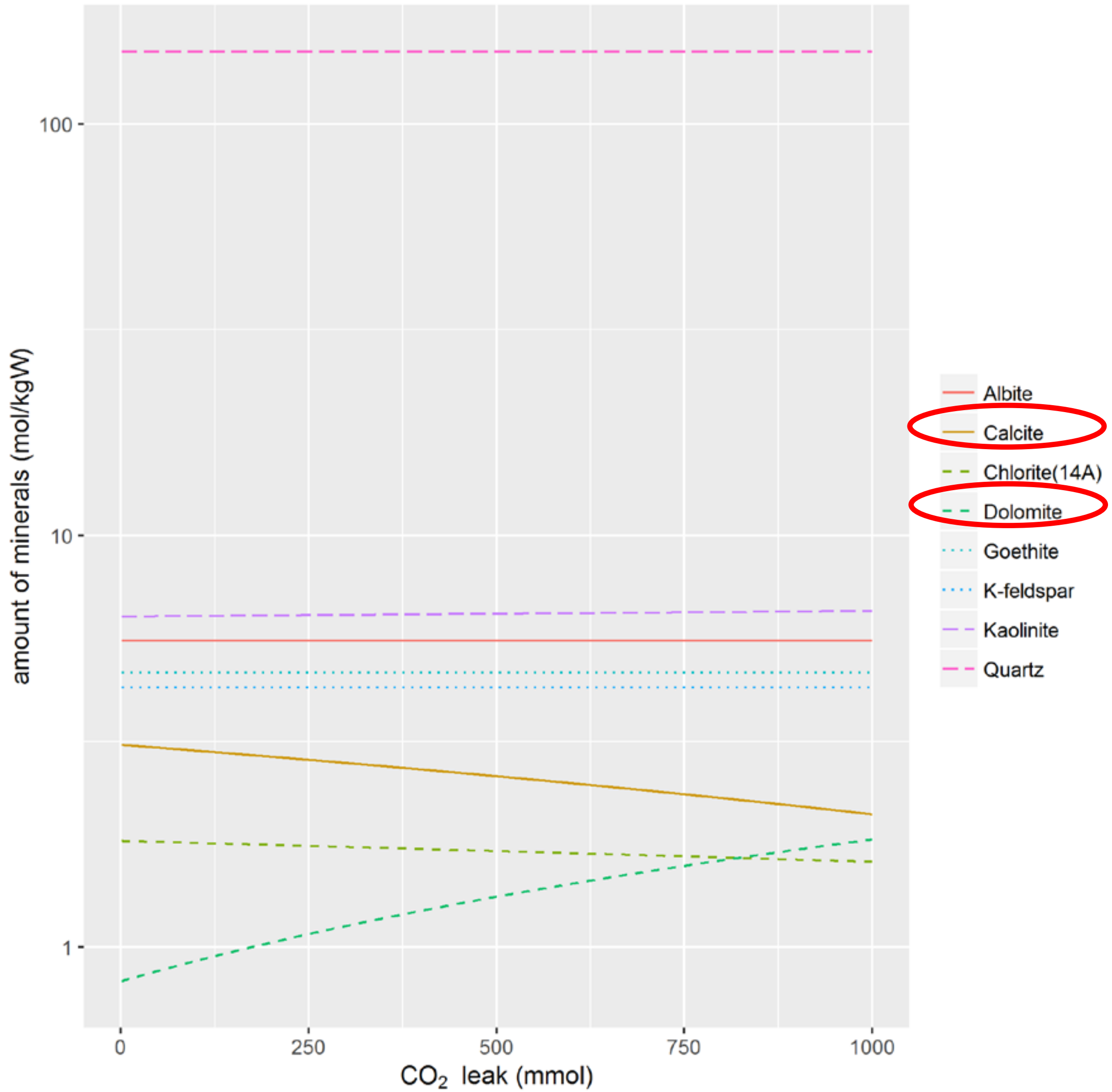
Showing 1 to 20 of 1,000 entries

	step	változó	value
992	992	Albite	5.5536
993	993	Albite	5.5536
994	994	Albite	5.5536
995	995	Albite	5.5536
996	996	Albite	5.5536
997	997	Albite	5.5536
998	998	Albite	5.5536
999	999	Albite	5.5535
1000	1000	Albite	5.5535
1001	1	Calcite	3.1017
1002	2	Calcite	3.1007
1003	3	Calcite	3.0997
1004	4	Calcite	3.0987
1005	5	Calcite	3.0977
1006	6	Calcite	3.0967
1007	7	Calcite	3.0957
1008	8	Calcite	3.0947
1009	9	Calcite	3.0937
1010	10	Calcite	3.0927
1011	11	Calcite	3.0917

Showing 992 to 1,011 of 8,000 entries

Thermodynamic mixing

CO_2 leaks into shallower **drinking water aquifer**



Thermodynamic mixing

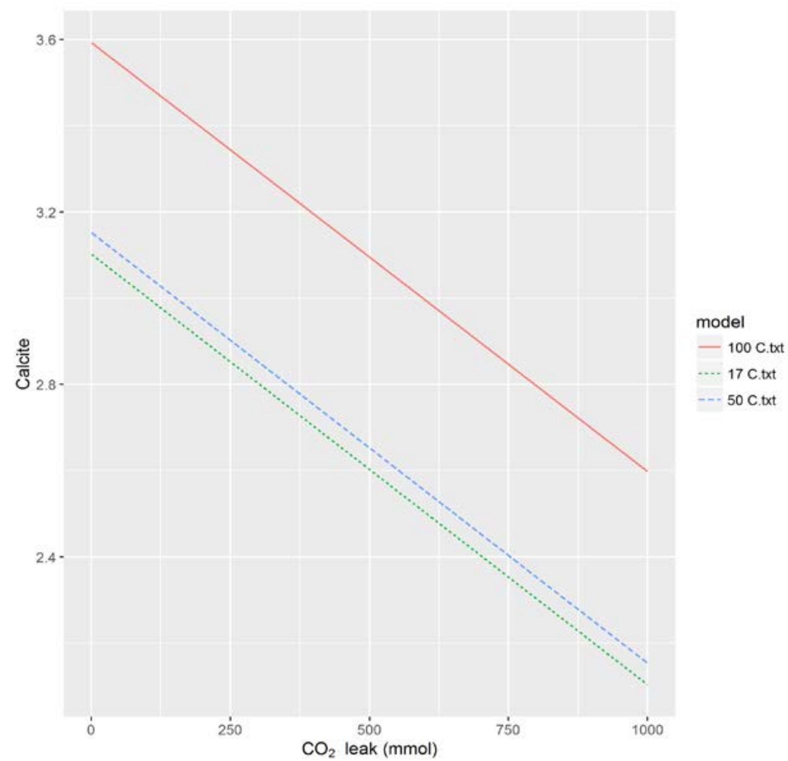
CO_2 leaks into shallower **drinking water aquifer**

```r
for (j in parameterList)
{
parameter<-j

#making an empty dataframe, first column is step
allData<-data.frame(step)

 for (i in files)
 {
  theFileName<-i
  dataInFiles<-read.table(theFileName, header=TRUE, fill=TRUE, check.names=FALSE)
  #dataInFiles$step[1]<-0
  dataInFiles<-filter(dataInFiles, step>=0)
  parameterData<-select(dataInFiles, one_of(parameter))
  names(parameterData)<-theFileName
  allData<-cbind(allData, parameterData)
 }

#figure name for given parameter
figname<-paste0("variation_", parameter, ".png")

#preparing the figure
toPlot<-melt(allData, id=c('step'))
names(toPlot)[2]<-"model"
plot<-ggplot(toPlot)
plot<-plot+geom_line(aes(x = step, y = value, colour = model,
plot<-plot+labs(x = xName, y = parameter)
ggsave(figname)
}
```

dplyr

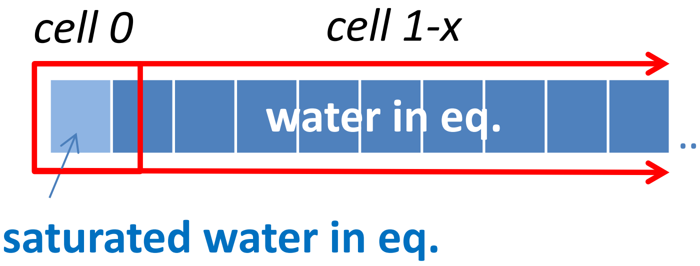
reshape2

ggplot2



Model sensitivity visualization
E.g. effect of temperature

1D reactive transport



cell time step

	sim	state	soln	dist_x	time	step	pH	pe	K	k_Calcite	dk_Calcite	k_Albite	dk_Albite
300	1	transp	95	94.5	10000	1	7.900041	-2.166457	0.010430075	1.469166	-0.005033613	5.724240	0.012239596
301	1	transp	96	95.5	10000	1	7.900041	-2.166457	0.010430075	1.469166	-0.005033613	5.724240	0.012239596
302	1	transp	97	96.5	10000	1	7.900041	-2.166457	0.010430075	1.469166	-0.005033613	5.724240	0.012239596
303	1	transp	98	97.5	10000	1	7.900041	-2.166457	0.010430075	1.469166	-0.005033613	5.724240	0.012239596
304	1	transp	99	98.5	10000	1	7.900041	-2.166457	0.010430075	1.469166	-0.005033613	5.724240	0.012239596
305	1	transp	100	99.5	10000	1	7.898592	-2.622879	0.010430908	1.469471	-0.004729498	5.724139	0.012139064
306	1	transp	1	0.5	20000	2	7.755056	-3.057924	0.008967509	2.246329	0.010024615	6.138284	0.003795477
307	1	transp	2	1.5	20000	2	7.888029	-3.178678	0.010759816	1.457187	-0.010159492	5.737782	0.013166106
308	1	transp	3	2.5	20000	2	7.924789	5.458658	0.012217597	1.476924	0.007435821	5.733691	0.009563021
309	1	transp	4	3.5	20000	2	7.929688	5.458670	0.012249935	1.477130	0.007963739	5.733721	0.009481848
310	1	transp	5	4.5	20000	2	7.930659	5.453108	0.012242591	1.477278	0.008111208	5.733698	0.009458110
311	1	transp	6	5.5	20000	2	7.930708	5.396017	0.012242326	1.477279	0.008112829	5.733698	0.009458019
312	1	transp	7	6.5	20000	2	7.930708	5.396017	0.012242326	1.477279	0.008112829	5.733698	0.009458019
313	1	transp	8	7.5	20000	2	7.930708	5.396017	0.012242326	1.477279	0.008112829	5.733698	0.009458019
314	1	transp	9	8.5	20000	2	7.930708	5.396017	0.012242326	1.477279	0.008112829	5.733698	0.009458019
315	1	transp	10	9.5	20000	2	7.930708	5.396017	0.012242326	1.477279	0.008112829	5.733698	0.009458019
316	1	transp	11	10.5	20000	2	7.930708	5.396017	0.012242326	1.477279	0.008112829	5.733698	0.009458019
317	1	transp	12	11.5	20000	2	7.930708	5.396017	0.012242326	1.477279	0.008112829	5.733698	0.009458019
318	1	transp	13	12.5	20000	2	7.930708	5.396017	0.012242326	1.477279	0.008112829	5.733698	0.009458019

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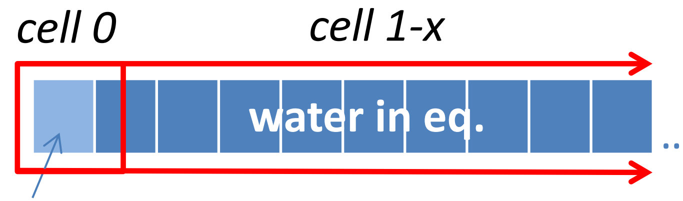
1D reactive transport

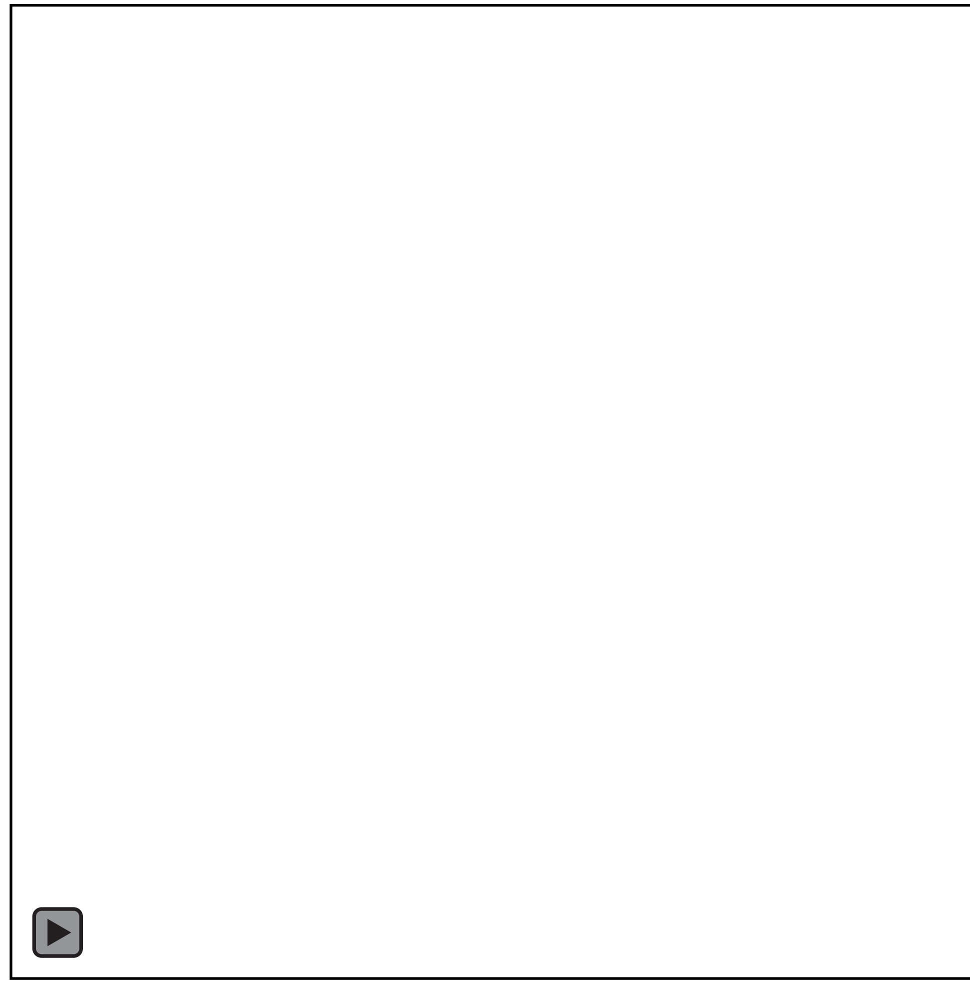


Synthetic Model Example

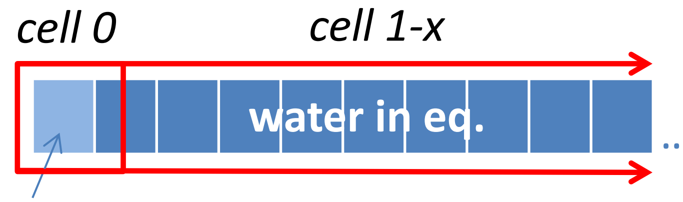
CO_2 saturated water in eq.

dplyr	reshape2	ggplot2	animation
select	melt	ggplot	saveVideo

```
stepn <- 0:50

asvanyData <- allData %>% select(soln, time, step, sta

gifnamemineral <- paste0(theFileName, "_minerals.mp4")

saveVideo({
  for(i in stepn){
    stepSubset <- asvanyData %>% filter(step==i) %>% s
    toGraph <- melt(stepSubset, id=c('soln'))
    linePlot <- ggplot(toGraph)
    linePlot <- linePlot + scale_y_continuous(limits =
    linePlot <- linePlot + geom_line(aes(x=soln, y=val
    linePlot <- linePlot + labs(title=paste("step", i)
    linePlot <- linePlot + labs(x="cell", y="concentra
    print(linePlot)
    ani.options(interval = 0.15)
  }
}, video.name = gifnamemineral)
```



1D reactive transport



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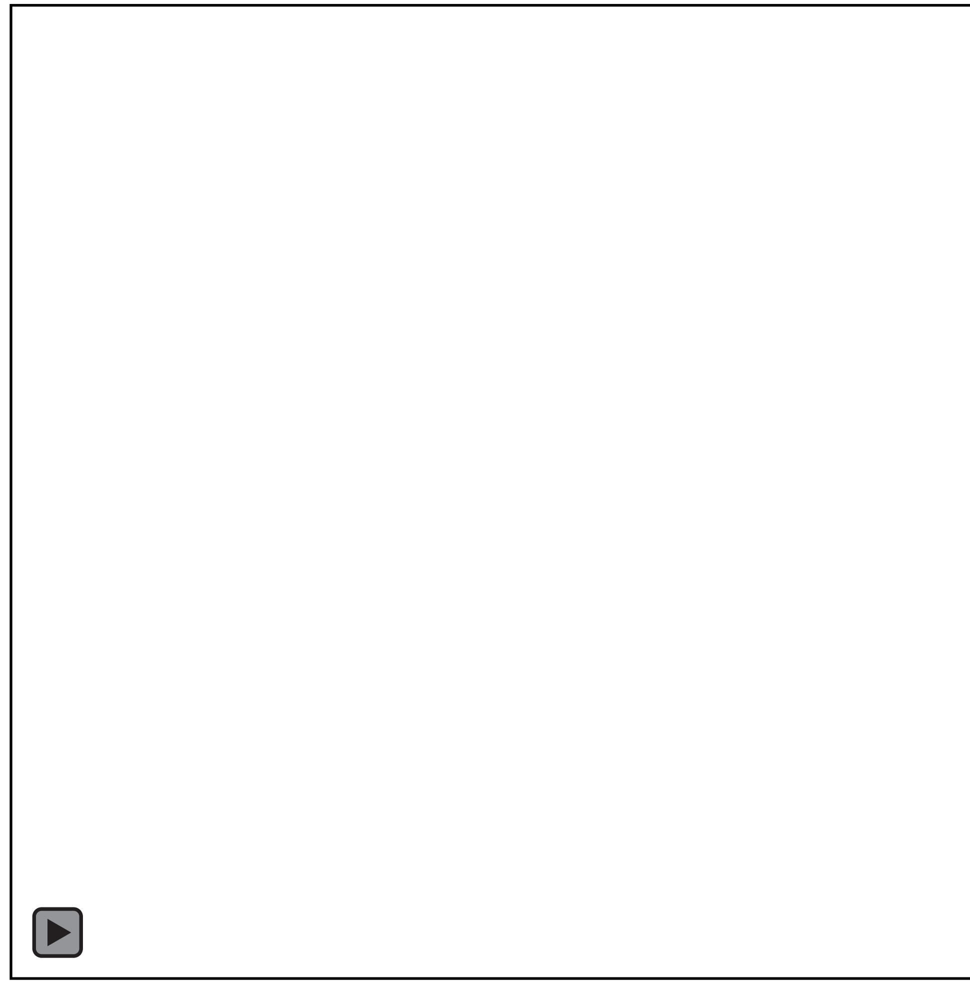


Package phreeqc and ReacTran

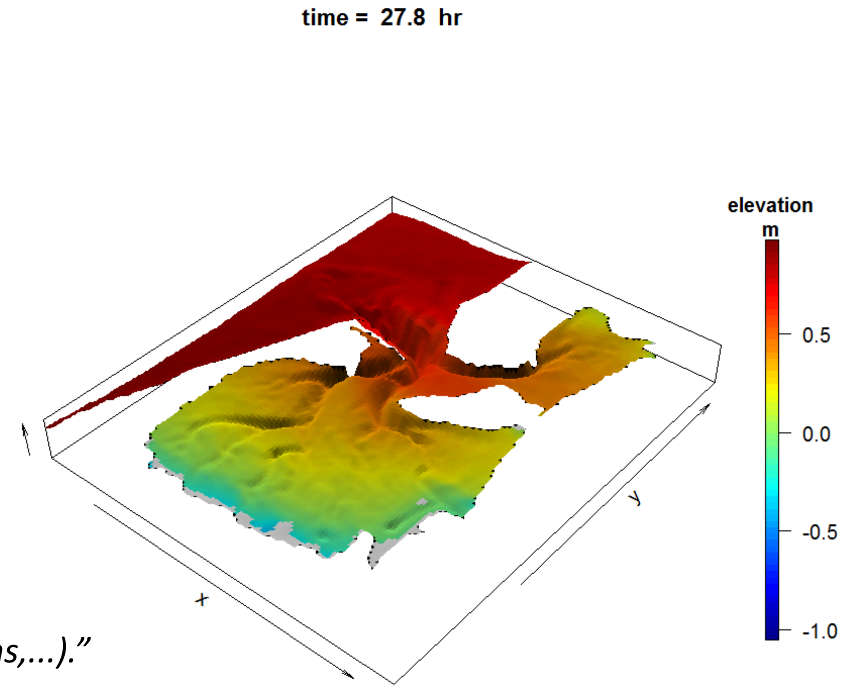
phreeqc - ***R Interface to Geochemical Modeling Software***
USGS, United States Geological Survey

ReacTran - ***Reactive transport modelling in 1D, 2D and 3D***
NIOZ, Royal Netherlands Institute for Sea Research

rootSolve
deSolve
shape

„ReacTran contains routines that enable the development of reactive transport models in

- *aquatic systems (rivers, lakes, oceans),*
- *porous media (floc aggregates, sediments,...) and*
- *idealized organisms (spherical cells, cylindrical worms,...).”*



https://www.nioz.nl/

Thank you for your attention!

Acknowledgements

György Falus, MFGI Project leader, PHREEQC
Nóra Gál, MFGI PHREEQC
Teodóra Szőcs, MFGI PHREEQC
Óskar Halldórsson Holm, Rittman Mead R
Online bloggers R, PHREEQC

EASAC 2013
Carbon capture and storage

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