

## SUPPORTING INFORMATION

### Monitoring of a simulated CO<sub>2</sub> leakage in a shallow aquifer using stable carbon isotopes

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Sampling campaigns, number of taken samples and the lowest measured isotope ratio of each campaign (SI-table 1/S1).

Isotope ratios and SF<sub>6</sub>-concentration of groundwater samples for all sampling campaigns (SI-table 2 / S1-S6).

Detailed information about the monitoring wells/ detailed description of the soil gas probe (S6)

Scheme of a self-constructed soil gas sampling lance. The Swagelok<sup>®</sup> valve on top is used as the sampling port. The percussion hammer is used to push the lance into the ground and to pull it out after the sampling (SI-figure 1/ S6).

Profile of one monitoring well with different sampling depths and a correlation with the distribution of isotope ratios in the specific depth (SI-figure 2/ S7).

**SI-table 1** Isotope ratios [‰] of soil gas for three sampling campaigns before and during the CO<sub>2</sub> injection.

Sampling point	May 2010	January 2011	February 2011	April 2011	May 2011
1C	-19.8	-17.9	-17.4	-19.5	-19.5
2C	-19.5	-18.2	-19.9	-28.1	-22.1
3C	-19.3	-17.0	-19.8	-17.7	-22.9
1D	n.m.	-21.6	-19.6	-20.1	-21.8
2D	n.m.	-18.6	-20.9	-26.9	-19.9
3D	n.m.	-23.2	-22.4	-19.8	-20.6
1E	-18.4	-19.9	-18.9	-19.2	-20.0
2E	-18.9	-18.0	-19.6	-20.3	-20.3
3E	-22.2	-22.2	-18.9	-21.3	-21.3
1F	-17.1	-18.7	-21.2	-21.7	n.m.
4F	-20.7	-17.8	-17.7	-19.3	-19.3
5F	-19.4	-20.5	-19.0	-19.2	-19.2
1A	-20.8	-20.7	-18.7	n.m.	n.m.

30 n.m. not measured

**SI-table 2** Sampling campaigns, number of samples and lowest measured  $\delta^{13}\text{C}$  value of  $\text{CO}_2$  in groundwater samples.

Campaign	Date	Lowest measured $\delta^{13}\text{C}$ value	Number of samples
-3	19.05.2010	$-23.05 \pm 0.06 \text{ ‰}$	5
-2	23.11.2010	$-24.62 \pm 0.22 \text{ ‰}$	21
-1	01. – 03.03.2011	$-22.01 \pm 0.14 \text{ ‰}$	43
0	23. – 25.03.2011	$-24.74 \pm 0.24 \text{ ‰}$	54
1	30. – 31.03.2011	$-24.53 \pm 0.47 \text{ ‰}$	39
2	01. – 02.04.2011	$-31.42 \pm 0.12 \text{ ‰}$	46
3	06. – 08.04.2011	$-30.82 \pm 0.17 \text{ ‰}$	46
4	11. – 13.04.2011	$-31.63 \pm 0.19 \text{ ‰}$	51
5	27. – 29.04.2011	$-31.79 \pm 0.02 \text{ ‰}$	60
6	10. – 12.05.2011	$-31.87 \pm 0.06 \text{ ‰}$	51
7	09. – 10.06.2011	$-31.57 \pm 0.02 \text{ ‰}$	40
8	28. – 30.06.2011	$-31.54 \pm 0.23 \text{ ‰}$	60
9	29. – 31.08.2011	$-30.87 \pm 0.37 \text{ ‰}$	59
10	17. – 20.10.2011	$-30.82 \pm 0.35 \text{ ‰}$	60

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32 **SI-table 3** Isotope ratios and  $\text{SF}_6$ -concentration of groundwater samples over the entire monitoring

33 campaign.

	18 m		15 m		12 m	
01.04.2011						
	$\delta^{13}\text{C}/^{12}\text{C} \text{ [‰]}$	$\text{SF}_6 \text{ [mg/L]}$	$\delta^{13}\text{C}/^{12}\text{C} \text{ [‰]}$	$\text{SF}_6 \text{ [mg/L]}$	$\delta^{13}\text{C}/^{12}\text{C} \text{ [‰]}$	$\text{SF}_6 \text{ [mg/L]}$
1A	-23.85	5	-23.85	5	-23.85	5
1D	-24.48	64	-24.48	64	-24.48	64

2D	-20.90	5	-20.90	5	-20.90	5
3D	-21.83	5	-21.83	5	-21.83	5
LUA	-21.27	5	-21.27	5	-21.27	5
ML1B	-21.18	5	-23.54	5	-22.91	5
ML1C	n.s.	n.s.	-31.42	28	-24.44	5
ML2C		n.m.	-20.92	5	-20.92	35
ML3C	-23.40	5	-23.16	5	-21.32	5
ZZ5		n.m.	-29.61	45		n.m.
06.04.2011						
1D	-26.76	150	-26.76	150	-26.76	150
2D	-22.45	5	-22.45	5	-22.45	5
3D	-23.00	5	-23.00	5	-23.00	5
LUA	-22.35	5	-22.35	5	-22.35	5
ML1B	-23.19	5	-22.39	5		n.m.
ML1C	n.s.	n.s.	-30.82	120	-24.40	5
ML2C	-21.68	5	-21.04	5	-29.87	540
ML3C	-23.03	5	-22.81	5	-22.15	5
ZZ3		n.m.	-20.81	5		n.m.
ZZ5	-25.05	140	-25.13	11	-25.19	120
ZZ6	n.s.	n.s.	-24.60	5	-24.60	5
11.04.2011						
1D	-29.09	180	-29.09	180	-29.09	180
2D	-22.28	17	-22.28	17	-22.28	17
1F	-21.90	5	-21.90	5	-21.90	5
4F	-19.80	5	-19.80	5	-19.80	5
5F	-22.58	5	-22.58	5	-22.58	5
LUA	-21.90	5	-21.90	5	-21.90	5

ML1B	-21.87	5	-21.93	5	-22.68	5
ML1C	n.s.	n.s.	-31.63	120	-26.07	9.2
ML1E	-20.23	5	-20.80	5	-23.67	5
ML2C	-31.64	530	-21.22	11	-30.44	720
ML2E	-20.44	5	-20.65	5	-20.71	5
ML3C	-22.78	5	-22.61	5	-22.37	5
ML3E	-22.10	5	-22.05	5	-22.44	5
ML8E	-20.08	5	-19.60	5	-19.75	5
ZZ3	-20.45	5	-20.66	5	-22.59	5
ZZ5	-27.21	390	-23.68	42	-28.53	580
ZZ6	n.s.	n.s.	-22.95	5	-22.99	5
10.05.2011						
1D	-30.62	200	-30.62	200		n.m.
2D		n.m.		n.m.	-28.56	98
3D	-28.56	98	-28.56	98	-31.50	220
ML1C	n.s.	n.s.	-32.57	270	-29.22	410
ML2C	-31.60	630	-22.41	5	-31.87	370
ML3C	-30.78	85	-23.97	390	-23.18	5
ML1E	-21.80	5	-22.52	5	-25.47	5
ML3E	-22.93	5	-21.82	5	-21.25	5
ML8E	-20.20	5		n.m.	-20.96	5
ML6F	-20.93	5	-22.13	5	-20.53	5
ML1G	-21.47	5	-23.28	5	n.s.	n.s.
ZZ1	-22.21	5	-22.21	5	-22.21	5
ZZ2	-19.53	5	-20.64	5	-30.62	200
ZZ3	-22.12	5	-20.76	5		n.m.
ZZ5	-21.07	5	-20.80	5	-22.91	5

ZZ6	-23.61	5	-24.16	5	-23.66	5
28.06.2011						
1A	-22.62	5.00	-22.62	5.00	-22.62	5.00
1D	-31.48	290.00	-31.48	290.00	-31.48	290.00
2D	-30.95	690.00	-30.95	690.00	-30.95	690.00
3D	-30.60	120.00	-30.60	120.00	-30.60	120.00
1F	-22.82	5	-22.82	5	-22.82	5
4F	-20.32	5.00	-20.32	5.00	-20.32	5.00
5F	-22.54	5.00	-22.54	5.00	-22.54	5.00
1H	-19.90	5.00	-19.90	5.00	-19.90	5.00
LUA	-30.82	270.00	-30.82	270.00	-30.82	270.00
ML1B	-22.00	5.00	-22.39	5.00	-22.13	5.00
ML1C	n.s.	n.s.	-28.22	480.00	-31.11	670.00
ML2C	-21.36	5.00	-31.49	300.00	-30.19	140.00
ML3C	-26.91	130	-24.31	5.00	-31.01	980
ML1E	-21.34	5.00	-31.42	180	-27.48	74.00
ML2E	-21.70	5.00	-21.88	5.00	-20.82	5
ML3E	-22.70	5.00	-31.55	450	-23.32	5.00
ML8E	-19.00	5.00	-19.19	5.00	-19.39	5.00
ML6F	-19.89	5.00	n.s.	n.s.	n.s.	n.s.
ZZ1	-22.27	5.00	-22.27	5.00	-22.27	5.00
ZZ2	-21.05	5.00	-20.75	5.00		n.m.
ZZ3	-20.59	5.00	-20.52	5.00	-22.29	5.00
ZZ5	-21.67	5.00	-21.40	5.00	-20.96	5.00
ZZ6	-22.84	5	-23.08	5.00	-22.80	5.00
30.08.2011						
1D	-28.74	350.00	-28.74	350.00	-28.74	350.00

2D	-28.21	180.00	-28.21	180.00	-28.21	180.00
3D	-26.50	100.00	-26.50	100.00	-26.50	100.00
1F	-25.28	57.00	-25.28	57.00	-25.28	57.00
4F	-20.37	5.00	-20.37	5.00	-20.37	5.00
5F	-25.92	49.00	-25.92	49.00	-25.92	49.00
LUA	-28.61	190.00	-28.61	190.00	-28.61	190.00
Z2	-22.39	5.00	-22.39	5.00	-22.39	5.00
ML1B	-22.83	5.00	-23.15	5.00	-23.03	5.00
ML1C	n.s.	n.s.	-25.48	110.00	-24.59	80.00
ML2C	-21.40	5.00	-25.61	110.00	-22.07	5.00
ML3C	-23.19	13.00	-23.62	5.00	-25.33	360.00
ML1E	-21.60	5.00	-28.53	230.00	-30.89	760.00
ML2E	-22.99	5.00	-21.08	5.00	-20.55	5.00
ML3E	-22.15	5.00	-30.28	800.00	-22.31	5.00
ZZ6	-22.36	5.00	-23.32	5.00	-22.32	5.00
19.10.2011						
1D	-23.61	68.00	-23.61	68.00	-23.61	68.00
2D	-22.33	29.00	-22.33	29.00	-22.33	29.00
3D	-25.17	37.00	-25.17	37.00	-25.17	37.00
1F	-29.61	230.00	-29.61	230.00	-29.61	230.00
4F	-21.34	5.00	-21.34	5.00	-21.34	5.00
5F	-27.62	95.00	-27.62	95.00	-27.62	95.00
1H	-19.73	5.00	-19.73	5.00	-19.73	5.00
LUA	-27.11	200.00	-27.11	200.00	-27.11	200.00
ML1B	-23.42	5.00	-23.11	5.00	-23.19	5.00
ML1C	n.s.	n.s.	-29.47	280.00	-22.30	7.40
ML2C	-21.40	5.00	-21.50	5.00	-23.13	5.00

ML3C	-23.04	5.50	-23.06	5.00	-22.11	8.30
ML1E	-25.91	58.00	-30.82	160.00	-30.55	650.00
ML2E	-30.82	44.00	-23.03	20.00	-21.07	5.00
ML3E	-30.82	44.00	-29.77	160.00	-25.15	35.00
ML1G	-19.77	5.00	-21.89	5.00	-21.40	5.00
ML6F	-19.73	5.00	-20.05	5.00	-19.93	5.00
ML8E	-19.96	5.00	-19.30	5.00	-20.09	5.00
ZZ1	-30.50	520.00	-30.50	520.00	-30.50	520.00
ZZ2	-20.14	5.00	-20.10	5.00	-20.14	5.00
ZZ3	-20.89	5.00	-20.31	5.00	-22.17	5.00
ZZ5	-20.85	5.00	-20.50	5.00	-20.68	5.00
ZZ6	-23.13	5.00	-24.36	5.00	-22.93	5.00

34

35 **Detailed information about the construction of the monitoring wells**

- 36 - 12 2" wells screened at 12-18 m bgl
- 37 - seven 1" wells screened at 12.5-13.5, 14.5-15.5 and 17.5-18.5 m bgl that were
- 38 separately sampled using a packer system
- 39 - 11 multi-level wells with different diameters and sampling points at 12, 15 and 18 m
- 40 bgl
- 41 - four sampling points at 12 m bgl
- 42 - one 4" well

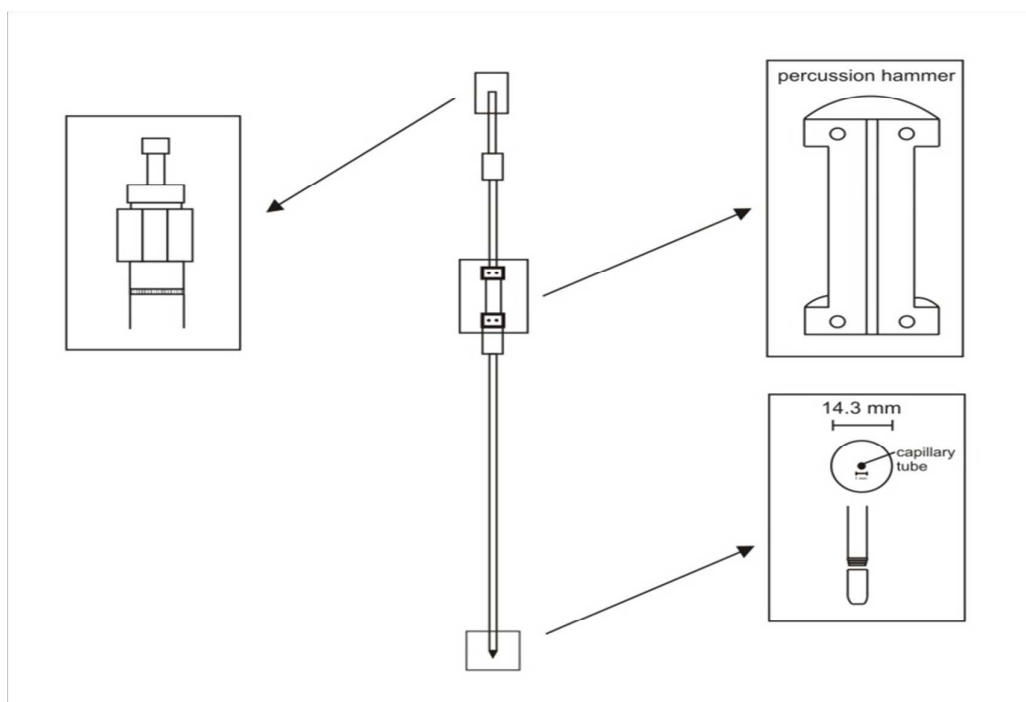
43 **Description of the soil gas probes**

44 A thin capillary tube with an inner diameter of 0.99 mm (outer diameter 3.8 mm) is placed in  
45 the middle of the lance. A small diameter was chosen in order to keep the death volume (1.1  
46 mL) as small as possible. On top of the lance a Swagelok<sup>®</sup> valve with a gas tight septum was  
47 used as sampling port. Before the lance was pushed into the ground, a metal rivet was placed

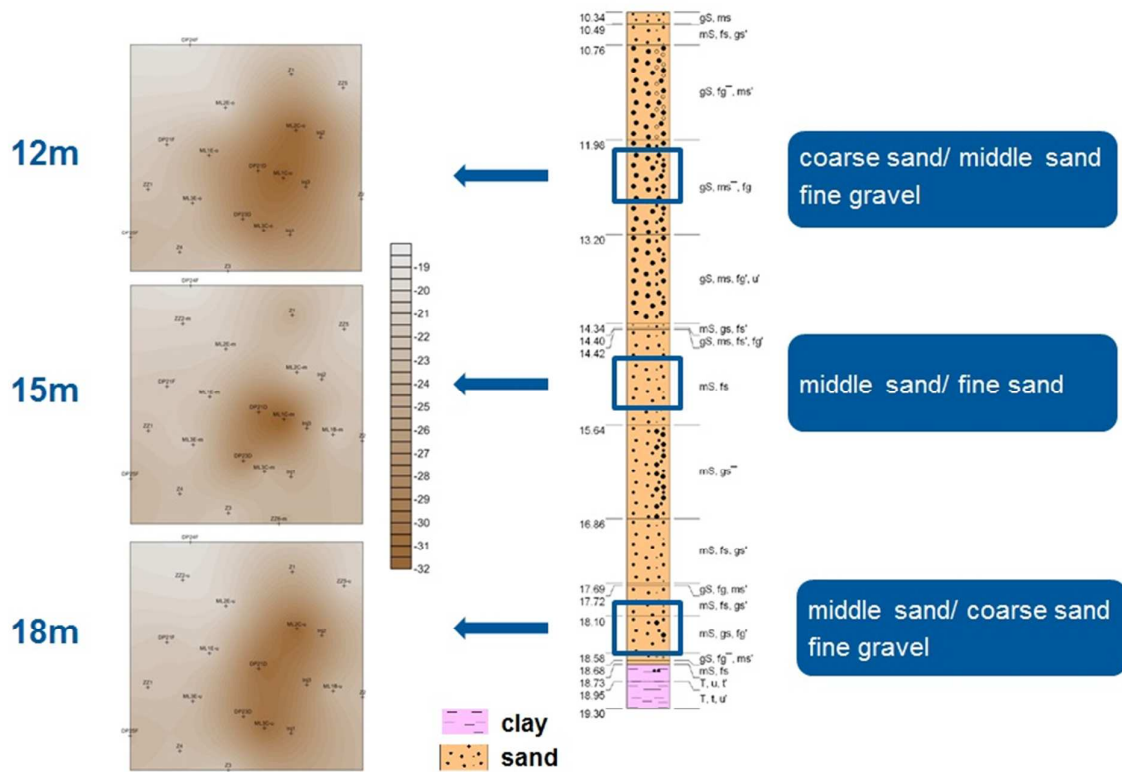


48 on the lower end of the lance to avoid a clogging of the capillary tube with sediments. The  
49 lance was pushed for about one meter manually into the ground. Afterwards, the lance was  
50 pulled about two centimeters out of the ground again, so that the rivet was lost and the lower  
51 end of the lance was open for sampling. A 5 mL gas-tight glass syringe (Hamilton, USA) was  
52 used to remove about five times the dead volume of the sampler from the capillary tube. The  
53 lances were left in the ground for at least 30 minutes to allow an equilibration of the soil gas  
54 before the samples were taken.

55



**SI-figure 1.** Scheme of the self-constructed soil gas sampling lances. The Swagelok<sup>®</sup> valve on the top is used as the sampling port. The percussion hammer is used to push the lance into the ground and to pull it out after the sampling.



**SI-figure 2.** Distribution of the isotope ratios correlated to the different depth of a profile of *MLC2*. It shows that the lithology has an influence on the distribution of the isotope ratios as coarse to middle sand has a higher pore space and therefore the isotopically light  $\text{CO}_2$  that is dissolved in the groundwater can migrate into a larger spatial area.