

APPENDICES

A1

Table A.1: Depth and thickness of the Trigonodus Dolomit and the Dolomit der Anhydritgruppe at all the wells investigated in this study.

Well	Depth TD (m)	Thickness TD (m)	Depth DAG (m)	Thickness DAG (m)	Basis for estimating lithological boundaries
Bözberg (BOZ)	58.4–96.0	37.6	136.0–148.8	12.8	DC
Böttstein (BOE)	121.9–150.8	28.9	197.2–204.6	7.4	Nagra, 1985
Siblingen (SIB)	177.0–207.8 ³	30.8	233.7–249.4	15.7	Nagra, 1992b
Riniken (RIN)	616.0–652.4	36.4	688.5–698.5	10.0	Nagra, 1990
Benken (BEN)	811.4–848.5	37.1	874.3–886.3	12.0	Nagra, 2001
Weiach (WEI)	819.1–857.1	38.0	887.9–897.7	9.8	Nagra, 1989
Schlattingen (SLA)	1112.0–1145.3	33.3	1169.5–1179.1	9.6	Diamond et al., 2013
Schafisheim (SHA)	1228.3–1256.3	28.0	1287.7–1305.0	17.3	Nagra, 1992a
Pfaffnau (PFA)	~ 1546–1575	~ 29.0	~ 1610–1622 ¹	~ 12.0	Büchi et al., 1965
Herdern (HER)	1990–2020	30.0	~ 2052–2062	~ 10.0	This study.
Berlingen (BER)	~ 2179–2191	~ 12.0	~ 2245–2257 ¹	~ 12.0	Büchi et al., 1965
Kreuzlingen (KRE)	~ 2415–2433 ²	~ 18.0	~ 2480–2492 ¹	~ 12.0	Büchi et al., 1965
Lindau (LIN)	~ 2225–2267 ²	~ 42.0	~ 2285–2297 ¹	~ 12.0	Büchi et al., 1965

TD: Trigonodus Dolomit; DAG: Dolomit der Anhydritgruppe

DC: drill core

¹ Exact depth of base of DAG cannot be determined precisely. Tabulated values are rough estimates.

² Exact depth of base of TD cannot be determined precisely. Tabulated values are minima based on our drill core investigations.

References:

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- Nagra (1992a) Sondierbohrung Schafisheim Untersuchungsbericht - Nagra Technischer Bericht NTB 88-11. Nagra, Wettingen, Switzerland.
- Nagra, 1992b. Sondierbohrung Siblingen Untersuchungsbericht - Nagra Technischer Bericht NTB 90-34. Nagra, Wettingen, Switzerland.

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Table A.2: Strontium isotope data for minerals and groundwater from various wells across the Swiss Molasse Basin.

Locality	Sample depth (m)	Phase	Occurrence	Unit	$^{87}\text{Sr}/^{86}\text{Sr}$	Sr ($\mu\text{g/g}$)
Benken	828.14	Dolomite	Rock matrix	TD	0.70844 ¹	89 ¹
Benken	836.46	Dolomite	Rock matrix	TD	0.70863 ¹	32 ¹
Schlattingen	1116.66	Dolomite	Rock matrix	TD	0.70886	45
Schlattingen	1121.87	Dolomite	Rock matrix	TD	0.70869	44
Schlattingen	1126.48	Dolomite	Rock matrix	TD	0.70979	35
Schlattingen	1127.83	Dolomite	Rock matrix	TD	0.71016	36
Schafisheim	1252.38	Dolomite	Rock matrix	TD	0.70967	–
Schafisheim	1233.93	Dolomite	Rock matrix	TD	0.70812 ²	85 ²
Böttstein	137.2	Dolomite	Rock matrix	TD	0.71053 ²	586 ²
Bözberg	64.82	Dolomite	Rock matrix	TD	0.70804	–
Bözberg	94.66	Dolomite	Rock matrix	TD	0.70876	–
Benken	853.98	Dolomite + Calcite	Rock matrix	HMK	0.70868 ¹	89 ¹
Schlattingen	1167.88	Dolomite + Calcite	Rock matrix	HMK	0.70824	198
Schlattingen	1168.31	Dolomite + Calcite	Rock matrix	HMK	0.70832	185
Bözberg	98.52	Dolomite + Calcite	Rock matrix	HMK	0.70919	–
Schafisheim	1334.99	Dolomite + Calcite	Rock matrix	HMK	0.70813	–
Weiach	828.57-1	Anhydrite	Nodules and beds	TD	0.70880	1026
Weiach	828.57-2	Anhydrite	Nodules and beds	TD	0.70872	977
Weiach	831.33-1	Anhydrite	Nodules and beds	TD	0.70876	1090
Weiach	831.33-2	Anhydrite	Nodules and beds	TD	0.70885	1144
Weiach	834.25	Anhydrite	Nodules and beds	TD	0.70860	1134
Weiach	824.85	Anhydrite	Nodules and beds	TD	0.70953 ²	2437 ²
Weiach	828.72	Anhydrite	Nodules and beds	TD	0.70874 ²	1222 ²
Schlattingen	1121.87	Anhydrite	Nodules and beds	TD	0.70846	1368
Schlattingen	1133.43	Anhydrite	Nodules and beds	TD	0.70900	1458
Schafisheim	1234.67	Anhydrite	Nodules and beds	TD	0.70822	–
Schafisheim	1294.17	Anhydrite	Nodules and beds	DAG	0.70805	–
Schafisheim	1295.76	Anhydrite	Nodules and beds	DAG	0.70804	–
Weiach	749.60	Anhydrite	Nodules and beds	Keuper	0.70821 ²	1893 ²
Böttstein	53.37	Anhydrite	Nodules and beds	Keuper	0.70811 ²	1576 ²
Böttstein	53.37	Anhydrite	Nodules and beds	Keuper	0.70814 ²	2150 ²
Böttstein	59.00	Anhydrite	Nodules and beds	Keuper	0.70810 ²	886 ²
Böttstein	88.90	Anhydrite	Nodules and beds	Keuper	0.70807 ²	2701 ²
Benken	730.76	Anhydrite	Nodules and beds	Keuper	0.70840 ¹	1896 ¹
Weiach	898.03	Anhydrite	Nodules and beds	Sulfatschichten	0.70798	1585
Weiach	904.43	Anhydrite	Nodules and beds	Sulfatschichten	0.70803	2746
Weiach	912.10	Anhydrite	Nodules and beds	Sulfatschichten	0.70796	1052
Weiach	923.27	Anhydrite	Nodules and beds	Sulfatschichten	0.70829	1570
Weiach	928.58	Anhydrite	Nodules and beds	Sulfatschichten	0.70806	1335
Weiach	937.74	Anhydrite	Nodules and beds	Sulfatschichten	0.70846	1420
Weiach	941.38	Anhydrite	Nodules and beds	Sulfatschichten	0.70845	2139
Weiach	943.12	Anhydrite	Nodules and beds	Sulfatschichten	0.70854	2056

Continuation of Table A.2

Locality	Sample depth (m)	Phase	Occurrence	Unit	$^{87}\text{Sr}/^{86}\text{Sr}$	Sr ($\mu\text{g/g}$)
Weiach	910.15	Anhydrite	Nodules and beds	Sulfatschichten	0.70783 ²	1105 ²
Schafisheim	1374.25	Anhydrite	Nodules and beds	Sulfatschichten	0.70785 ²	1142 ²
Leuggern	116.43	Anhydrite	Nodules and beds	Sulfatschichten	0.70784 ²	1196 ²
Böttstein	122.65	Calcite	Pore-filling	TD	0.70936 ²	100 ²
Böttstein	150.99	Calcite	Fracture-filling	TD	0.70877	–
Leuggern	54.08	Calcite	Pore-filling	TD	0.70905 ²	58 ²
Benken	846.46-1	Calcite	Shear surface	TD	0.70865 ¹	61 ¹
Benken	846.46-2	Calcite	Pore-filling	TD	0.70839 ¹	34 ¹
Schafisheim	1252.77-1	Calcite	Pore-filling	TD	0.70882	–
Schafisheim	1252.77-2	Calcite	Pore-filling	TD	0.70858	–
Weiach	844.99	Calcite	Pore-filling	TD	0.71016	–
Weiach	861.58	Calcite	Pore-filling	HMK	0.70929	–
Benken	853.98	Calcite	Fracture-filling	HMK	0.71079 ¹	105 ¹
Benken	866.41	Calcite	Pore-filling	HMK	0.71123	133
Benken	866.42	Calcite	Pore-filling	HMK	0.71137	110
Benken	866.44	Calcite	Pore-filling	HMK	0.71090	67
Benken	866.46	Calcite	Pore-filling	HMK	0.71173	139
Schlattingen	1157.34	Calcite	Pore-filling	HMK	0.71629	204
Schlattingen	1164.33	Calcite	Pore-filling	HMK	0.70964	1924
Schlattingen	1167.88	Calcite	Fracture-filling	HMK	0.71289	197
Schlattingen	1168.31	Calcite	Pore-filling	HMK	0.71260	169
Schafisheim	1329.20	Calcite	Fracture-filling	HMK	0.70966 ²	233 ²
Schafisheim	1285.34	Calcite	Tension gash	HMK	0.70965	–
Schafisheim	1330.70	Calcite	Fracture-filling	HMK	0.70959	–
Schafisheim	1334.99	Calcite	Fracture-filling	HMK	0.70968	–
Bözberg	98.52	Calcite	Fracture-filling	HMK	0.70838	–
Bözberg	135.69	Calcite	Fracture-filling	HMK	0.71231	–
Siblingen	209.95	Calcite	Pore-filling	HMK	0.70945	–
Benken	878.25	Calcite	Fracture-filling	DAG	0.71023 ¹	1098 ¹
Bözberg	147.61	Calcite	Fracture-filling	DAG	0.70855	–
Böttstein	196.94	Calcite	Pore-filling	DAG	0.71213	–
Siblingen	241.60	Calcite	Fracture-filling	DAG	0.70938	–
Benken	401.68	Calcite	Fracture-filling	Jurassic	0.70712 ¹	231 ¹
Benken	519.96	Calcite	Fracture-filling	Jurassic	0.70763 ¹	–
Benken	635.67	Calcite	Fracture-filling	Jurassic	0.70847 ¹	283 ¹
Benken	657.62	Calcite	Pore-filling	Jurassic	0.70758 ¹	342 ¹
Benken	712.76	Calcite	Fracture-filling	Keuper	0.70925 ¹	189 ¹
Benken	713.26	Calcite	Fracture-filling	Keuper	0.70921 ¹	296 ¹
Schafisheim	1485.75	Calcite	Fracture-filling	Buntsandstein	0.71300 ²	3566 ²
Riniken	805.00	Calcite	Pore-filling	Buntsandstein	0.71504 ²	290 ²
Leuggern	218.61	Calcite	Pore-filling	Buntsandstein	0.71659 ²	107 ²
Riniken	1045.45	Calcite	Fracture-filling	Permian	0.71618 ²	286 ²
Kaisten	1046.36	Calcite	Fracture-filling	CB	0.71701 ²	148 ²
Leuggern	1511.32	Calcite	Fracture-filling	CB	0.71156 ²	–

Continuation of Table A.2

Locality	Sample depth (m)	Phase	Occurrence	Unit	$^{87}\text{Sr}/^{86}\text{Sr}$	Sr ($\mu\text{g/g}$)
Leuggern	1525.97	Calcite	Fracture-filling	CB	0.71105 ²	–
Leuggern	318.65	Calcite	Fracture-filling	CB	0.71129	–
Siblingen	1023.62	Calcite	Fracture-filling	CB	0.71535	–
Benken	998.99	Calcite	Fracture-filling	CB	0.71111	–
Schlattingen	1116.66-1	Anhydrite	Fracture-filling	TD	0.71035	1876
Schlattingen	1116.66-2	Anhydrite	Fracture-filling	TD	0.70987	1616
Schlattingen	1135.58	Anhydrite	Pore-filling	TD	0.71048	2082
Schlattingen	1136.98	Anhydrite	Pore-filling	TD	0.70880	1562
Schlattingen	1127.83	Anhydrite	Fracture-filling	TD	0.70897	966
Schlattingen	1135.29	Anhydrite	Pore-filling	TD	0.70928	182
Schlattingen	1140.15	Anhydrite	Pore-filling	TD	0.71004	742
Schafisheim	1228.45	Anhydrite	Fracture-filling	TD	0.70983	–
Schafisheim	1330.70	Anhydrite	Fracture-filling	HMK	0.70951	–
Schafisheim	1334.99	Anhydrite	Fracture-filling	HMK	0.70995	–
Berlingen	2189.45	Saddle dolomite	Pore-filling	TD	0.71273	–
Berlingen	2189.01	Saddle dolomite	Pore-filling	TD	0.71239	–
Berlingen	2180.64	Saddle dolomite	Pore-filling	TD	0.71330	–
Berlingen	2181.37	Saddle dolomite	Pore-filling	TD	0.71324	–
Berlingen	2189.11	Saddle dolomite	Pore-filling	TD	0.71227	–
Berlingen	2179.87	Saddle dolomite	Pore-filling	TD	0.71313	–
Lindau	2245.35	Saddle dolomite	Pore-filling	TD	0.71217	–
Lindau	2232.64	Saddle dolomite	Pore-filling	TD	0.71219	–
Kreuzlingen	2422.75	Saddle dolomite	Pore-filling	TD	0.71313	–
Kreuzlingen	2431.39	Saddle dolomite	Pore-filling	TD	0.71306	–
Kreuzlingen	2427.18	Saddle dolomite	Pore-filling	TD	0.71338	–
Kreuzlingen	2422.95	Saddle dolomite	Pore-filling	TD	0.71339	–
Herdern	1990.01	Saddle dolomite	Pore-filling	TD	0.71280	–
Herdern	1995.57	Saddle dolomite	Pore-filling	TD	0.71265	–
Herdern	1998.93	Saddle dolomite	Pore-filling	TD	0.71233	–
Böttstein	1490.70	Rock matrix	Whole rock	CB	0.72716 ²	207 ²
Weiach	2220.12	Rock matrix	Whole rock	CB	0.71441 ²	244 ²
Kaisten	1038.83	Rock matrix	Whole rock	CB	0.72392 ²	–
Kaisten	1046.36	Rock matrix	Whole rock	CB	0.72305 ²	–
Leuggern	1525.97	Rock matrix	Whole rock	CB	0.72859 ²	206 ²
Leuggern	1636.90	Rock matrix	Whole rock	CB	0.76098 ²	290 ²
Schafisheim	1879.79	Rock matrix	Whole rock	CB	0.71405 ²	494 ²
Benken	396.62	Rock matrix	Whole rock	Malm	0.70704 ¹	385 ¹
Benken	401.68	Rock matrix	Whole rock	Malm	0.70708 ¹	390 ¹
Benken	519.96	Rock matrix	Whole rock	Dogger	0.70743 ¹	216 ¹
Benken	545.16	Rock matrix	Whole rock	Dogger	0.70784 ¹	179 ¹
Benken	571.55	Rock matrix	Whole rock	Dogger	0.70773 ¹	256 ¹
Benken	582.09	Rock matrix	Whole rock	Dogger	0.70789 ¹	163 ¹
Benken	635.67	Rock matrix	Whole rock	Dogger	0.70818 ¹	134 ¹
Benken	645.05	Rock matrix	Whole rock	Dogger	0.70808 ¹	203 ¹

Continuation of Table A.2

Locality	Sample depth (m)	Phase	Occurrence	Unit	$^{87}\text{Sr}/^{86}\text{Sr}$	Sr ($\mu\text{g/g}$)
Benken	657.62	Rock matrix	Whole rock	Liassic	0.70747 ¹	678 ¹
Benken	683.27	Rock matrix	Whole rock	Liassic	0.70911 ¹	112 ¹
Benken	702.37	Rock matrix	Whole rock	Keuper	0.70902 ¹	1033 ¹
Benken	712.76	Rock matrix	Whole rock	Keuper	0.70864 ¹	513 ¹
Benken	713.26	Rock matrix	Whole rock	Keuper	0.70879 ¹	1099 ¹
Benken	730.76	Rock matrix	Whole rock	Keuper	0.70889 ¹	88 ¹
Böttstein	123–202	Water	Groundwater	UMK	0.70968 ²	11 ²
Benken	813–826	Water	Groundwater	UMK	0.70830 ¹	6.5 ¹
Weiach	822–896	Water	Groundwater	UMK	0.70881 ²	7.9 ²
Schafisheim	1227–1293	Water	Groundwater	UMK	0.70919 ²	17.2 ²
Riniken	617–696	Water	Groundwater	UMK	0.70924 ²	13.6 ²
Leuggern	53–96	Water	Groundwater	UMK	0.70867 ²	3.1 ²
Weiach	981–989	Water	Groundwater	Buntsandstein	0.71652 ²	11.3 ³
Böttstein	305–319	Water	Groundwater	Buntsandstein	0.71455 ²	0.9 ²
Schafisheim	1476–1500	Water	Groundwater	Buntsandstein	0.71343 ²	17.8 ³
Schafisheim	1564–1577	Water	Groundwater	Buntsandstein	0.71442 ²	0.5 ²
Riniken	793–820	Water	Groundwater	Buntsandstein	0.71506 ²	16.0 ³
Kaisten	617–696	Water	Groundwater	Buntsandstein	0.71386 ²	12.6 ²
Leuggern	208–227	Water	Groundwater	Buntsandstein	0.71629 ²	0.7 ²
Benken	974–983	Water	Groundwater	Buntsandstein	0.71485 ¹	0.3 ¹
Böttstein	393–405	Water	Groundwater	CB	0.71730 ²	0.4 ²
Böttstein	618–624	Water	Groundwater	CB	0.71752 ²	0.1 ³
Weiach	2211–2224	Water	Groundwater	CB	0.71671 ²	4.7 ²
Schafisheim	1883–1892	Water	Groundwater	CB	–	16.2 ³
Leuggern	507–568	Water	Groundwater	CB	0.71672 ²	0.5 ²
Leuggern	702–709	Water	Groundwater	CB	0.71656 ²	0.5 ²
Leuggern	1179–1227	Water	Groundwater	CB	0.71729 ²	0.3 ²
Leuggern	1427–1439	Water	Groundwater	CB	0.71741 ²	0.7 ²
Leuggern	1642–1688	Water	Groundwater	CB	0.71747 ²	0.4 ²
Kaisten	475–489	Water	Groundwater	CB	0.71722 ²	1.5 ³
Kaisten	816–822	Water	Groundwater	CB	0.71767 ²	1.3 ²
Kaisten	1021–1040	Water	Groundwater	CB	0.71778 ²	1.4 ²
Kaisten	1238–1305	Water	Groundwater	CB	0.71711 ²	1.0 ²
Bruche	–	Water	River water	CB dominated	0.71051 ⁴	0.04 ⁴
Geissen	–	Water	River water	CB dominated	0.71639 ⁴	0.03 ⁴
Weiss	–	Water	River water	CB dominated	0.71692 ⁴	0.03 ⁴
Fecht	–	Water	River water	CB dominated	0.71330 ⁴	0.03 ⁴
Lauch	–	Water	River water	CB dominated	0.70906 ⁴	0.04 ⁴
Thur	–	Water	River water	CB dominated	0.71015 ⁴	0.03 ⁴
Doller	–	Water	River water	CB dominated	0.70913 ⁴	0.03 ⁴
Murg	–	Water	River water	CB dominated	0.71414 ⁴	0.02 ⁴
Kinzig	–	Water	River water	CB dominated	0.71413 ⁴	0.04 ⁴
Elz-1	–	Water	River water	CB dominated	0.71096 ⁴	0.10 ⁴
Elz-2	–	Water	River water	CB dominated	0.71306 ⁴	0.03 ⁴

Continuation of Table A.2

Locality	Sample depth (m)	Phase	Occurrence	Unit	$^{87}\text{Sr}/^{86}\text{Sr}$	Sr ($\mu\text{g/g}$)
Vosges	—	Water	Shallow GW	CB	0.71267 ⁴	0.91 ⁴
Vosges	—	Water	Shallow GW	CB	0.71571 ⁴	0.06 ⁴
Black Forest	—	Water	Shallow GW	CB	0.71393 ⁴	0.09 ⁴
Black Forest	—	Water	Shallow GW	CB	0.71381 ⁴	0.07 ⁴
Nettenbach	—	Water	Shallow GW	OSM	0.70963 ⁵	—
Stahringen	—	Water	Shallow GW	OSM	0.70961 ⁵	—
Hemmenhofen	—	Water	Shallow GW	OSM	0.70949 ⁵	—
Bankholzen	—	Water	Shallow GW	OSM	0.70938 ⁵	—
Horn	58–82	Water	Shallow GW	OSM	0.70929 ⁵	—
Gundholzen	—	Water	Shallow GW	OSM	0.70905 ⁵	—
—	—	Water	Shallow GW	OSM–UMM	0.7079–0.7091 ⁶	—

TD: Trigonodus Dolomit

HMK: Hauptmuschelkalk

DAG: Dolomit der Anhydritgruppe

CB: Crystalline basement

OSM: Upper Freshwater Molasse

UMM: Lower Seawater Molasse

¹ Nagra [38]² Pearson et al. [20]³ Wittwer [61]⁴ Durand et al. [40]⁵ Waber et al. [21]⁶ McArthur et al. [39]

A3

Table A.3: Compilation of microthermometric analyses of primary fluid inclusions in secondary minerals from various wells across the Swiss Molasse Basin.

Well	Sample ID	Mineral	Occurrence	Unit	Trapping mode	Analysed assemblages	T_{trap} (° C)	$T_{m,ice}$ (° C)	Salinity (wt.% NaCl _{eq})
Benken	BEN 825.11	Quartz	Pore-filling	TD	Heterogeneous (aq. liquid + CH ₄ gas)	1	52	-22.3 to -0.7	1.2–23.9*
Benken	BEN 828.14	Quartz	Pore-filling	TD	Heterogeneous (aq.liquid + CH ₄ gas)	3	41–47	-21.0 to -6.2	9.5–23.0*
Schlattingen	SLA 1126.46	Quartz	Pore-filling	TD	Heterogeneous (aq.liquid + CH ₄ gas)	6	42–58	-20.9 to -2.1	3.5–23.0*
Schlattingen	SLA 1127.44	Quartz	Pore-filling	TD	Heterogeneous (aq.liquid + CH ₄ gas)	4	42–48	-21.9 to -3.7	6.0–23.6*
Benken	BEN 866.44	Calcite	Pore-filling	HMK	Heterogeneous (aq.liquid + CH ₄ gas)	5	85–88	-1.9 to -0.2	0.4–3.2
Benken	BEN 998.99	Calcite	Fracture-filling	CB	Heterogeneous (aq.liquid + CH ₄ gas)	2	55–62	-28.6 to -20.2	22.5–27.8*
Schlattingen	SLA 1127.83	Calcite	Fracture-filling	TD	Heterogeneous (aq.liquid + CH ₄ gas)	1	80	-1.0 to -0.1	0.2–2.7
Schlattingen	SLA 1135.29	Calcite	Pore-filling	TD	Heterogeneous (aq.liquid + CH ₄ gas)	1	89	-2.9 to -1.5	2.6–4.8
Schlattingen	SLA 1157.34	Calcite	Pore-filling	HMK	Heterogeneous (aq.liquid + CH ₄ gas)	1	76	-3.4	5.6
Schlattingen	SLA 1167.88	Calcite	Fracture-filling	HMK	Heterogeneous (aq.liquid + CH ₄ gas)	1	78	-4.0 to -3.1	5.1–6.5
Siblingen	SIB 241.60	Calcite	Fracture-filling	HMK	Heterogeneous (aq.liquid + CH ₄ gas)	3	65–75	-0.1 to -1.7	0.2–2.9
Siblingen	SIB 1023.62	Calcite	Fracture-filling	CB	Heterogeneous (aq.liquid + CH ₄ gas)	3	65–75	-0.1 to -0.3	0.2–0.5
Leuggern	LEU 318.65	Calcite	Fracture-filling	CB	Heterogeneous (aq.liquid + CH ₄ gas)	2	85–95	-28.7 to -21.1	23.1–27.8*
Böttstein	BOE 150.99	Calcite	Fracture-filling	TD	Heterogeneous (aq.liquid + CH ₄ gas)	3	51–55	-12.7 to -17.7	16.6–20.7
Bözberg	BOZ 98.52	Calcite	Fracture-filling	HMK	Heterogeneous (aq.liquid + CH ₄ gas)	2	68–79	-23.7 to -15.2	18.8–24.9*
Schafisheim	SHA 1285.34	Calcite	Tension gash	HMK	Heterogeneous (aq.liquid + CH ₄ gas)	4	75–85	-12.3 to -4.0	6.5–16.3
Schafisheim	SHA 1252.77	Calcite	Pore-filling	TD	Heterogeneous (aq.liquid + CH ₄ gas)	3	52–65	-22.5 to -5.1	8.0–24.1*
Schafisheim	SHA 1334.99	Calcite	Fracture-filling	DAG	Heterogeneous (aq.liquid + CH ₄ gas)	1	65	-21.4 to -6.4	9.7–23.4*
Schafisheim	SHA 1252.38	Calcite	Pore-filling	TD	Heterogeneous (aq.liquid + CH ₄ gas)	1	65	-22.5 to -5.0	7.9–24.1*
Lindau	LIN 2245.35	Saddle dolomite	Pore-filling	TD	Homogeneous (aq. liquid)	6	155–161**	-4.8 to -3.1	5.1–7.6
Berlingen	BER 2189.11	Saddle dolomite	Pore-filling	TD	Homogeneous (aq. liquid)	5	152–156**	-4.2 to -2.1	3.6–6.7

HMK: Hauptmuschelkalk

DAG: Dolomit der Anhydritgruppe

CB: Crystalline basement

T_{trap} : Fluid inclusion trapping temperature

$T_{m,ice}$: Final ice melting temperature

Salinities are calculated according to Hall et al. [44]

*: The measured final ice melting temperatures below the eutectic temperature of NaCl-H₂O fluids (-21.2 °C; [44]) indicate that the corresponding parent-water contained other salts beside NaCl. The presence of Ca and Mg in the host rocks point towards additional CaCl₂ and MgCl₂.

** Pressure corrected fluid inclusion trapping temperatures.

A4

Table A.4: Results of the oxygen isotope analyses and calculated parent-waters of secondary quartz, calcite and dolomite from various wells across the Swiss Molasse Basin.

Well	Sample depth (m)	Mineral	Occurrence	Unit	$\delta^{18}\text{O}_{\text{mineral}}$ (‰ VSMOW)	T_{trap} (° C)	$\delta^{18}\text{O}_{\text{parent-water}}$ (‰ VSMOW)
Benken	825.11-1	Quartz	Pore-filling	TD	27.3	41–52	-4.6 to -2.1
Benken	825.11-2	Quartz	Pore-filling	TD	27.3	41–52	-4.6 to -2.1
Benken	825.11-3	Quartz	Pore-filling	TD	25.9	41–52*	-6.0 to -3.5
Benken	825.11-4	Quartz	Pore-filling	TD	25.5	41–52	-6.4 to -3.9
Benken	828.14-1	Quartz	Pore-filling	TD	25.1	41–52	-6.8 to -4.3
Benken	828.14-2	Quartz	Pore-filling	TD	27.3	41–52*	-4.6 to -2.1
Benken	828.14-3	Quartz	Pore-filling	TD	26.4	41–52	-5.5 to -3.0
Benken	828.14-4	Quartz	Pore-filling	TD	26.0	41–52	-5.9 to -3.4
Benken	839.81-1	Calcite	Pore-filling	TD	15.2	85–88	-3.6 to -3.2
Benken	839.81-2	Calcite	Pore-filling	TD	15.0	85–88	-3.8 to -3.4
Benken	833.87	Calcite	Pore-filling	TD	15.5	85–88	-3.3 to -3.0
Benken	866.41	Calcite	Pore-filling	HMK	14.4	85–88	-4.4 to -4.0
Benken	866.42	Calcite	Pore-filling	HMK	15.0	85–88	-3.8 to -3.4
Benken	866.44	Calcite	Pore-filling	HMK	14.0	85–88*	-4.8 to -4.4
Benken	866.45	Calcite	Pore-filling	HMK	15.3	85–88	-3.5 to -3.1
Benken	866.46	Calcite	Pore-filling	HMK	14.0	85–88	-4.8 to -4.4
Benken	866.47	Calcite	Pore-filling	HMK	15.5	85–88	-3.3 to -2.9
Benken	866.49	Calcite	Pore-filling	HMK	13.9	85–88	-4.9 to -4.5
Benken	998.99	Calcite	Fracture-filling	CB	22.0	55–62*	-0.9 to 0.1
Bözberg	98.52	Calcite	Fracture-filling	HMK	24.3	68–79	3.3 to 4.8
Bözberg	105.20	Calcite	Fracture-filling	HMK	19.6	68–79*	-1.4 to 0.1
Bözberg	135.69	Calcite	Fracture-filling	DAG	18.4	68–79	-2.6 to -1.1
Schlattingen	1157.34	Calcite	Pore-filling	HMK	15.2	76*	-4.7
Schlattingen	1167.88	Calcite	Fracture-filling	HMK	14.8	78*	-4.9
Schlattingen	1168.31	Calcite	Pore-filling	HMK	14.1	76–89	-5.9 to -4.3
Schlattingen	1170.48	Calcite	Fracture-filling	DAG	13.9	76–89	-6.0 to -4.4
Schlattingen	1171.00	Calcite	Fracture-filling	DAG	14.7	76–89	-5.2 to -3.6
Schlattingen	1177.10	Calcite	Pore-filling	DAG	13.5	76–89	-6.4 to -4.8
Schafisheim	1252.77	Calcite	Fracture-filling	TD	26.2	52–65*	2.8 to 4.8
Schafisheim	1285.34	Calcite	Tension gash	HMK	24.6	75–85*	4.6 to 5.9
Schafisheim	1327.06	Calcite	Fracture-filling	DAG	25.8	65	4.3
Schafisheim	1330.70	Calcite	Fracture-filling	DAG	22.6	65	1.1
Schafisheim	1334.99	Calcite	Fracture-filling	DAG	24.1	65*	2.7
Böttstein	146.31	Calcite	Pore-filling	TD	17.8	51–55	-5.8 to -5.2
Böttstein	150.99	Calcite	Fracture-filling	TD	20.9	51–55*	-2.7 to -2.1
Böttstein	196.94	Calcite	Pore-filling	HMK	16.3	51–55	-7.2 to -6.6
Siblingen	244.72	Calcite	Pore-filling	DAG	15.6	65–75	-5.8 to -4.5
Siblingen	241.60	Calcite	Fracture-filling	DAG	17.4	65–75*	-4.1 to -2.7
Siblingen	209.95	Calcite	Pore-filling	HMK	18.9	65–75	-2.5 to -1.1
Siblingen	242.37	Calcite	Fracture-filling	DAG	17.1	65–75	-4.3 to -2.9
Lindau	2250.14	Saddle dolomite	Pore-filling	TD	23.6	>141–147	8.5 to 9.0
Lindau	2232.64	Saddle dolomite	Pore-filling	TD	21.2	>141–147	6.1 to 6.6
Lindau	2245.35	Saddle dolomite	Pore-filling	TD	21.9	>141–147*	6.7 to 7.2
Lindau	2249.42	Saddle dolomite	Pore-filling	TD	23.5	>141–147	8.3 to 8.8

Continuation of Table A.4

Well	Sample depth (m)	Mineral	Occurrence	Unit	$\delta^{18}\text{O}_{\text{mineral}}$ (‰ VSMOW)	T_{trap} (° C)	$\delta^{18}\text{O}_{\text{parent-water}}$ (‰ VSMOW)
Berlingen	2179.87	Saddle dolomite	Pore-filling	TD	13.7	>138–142	-1.8 to -1.4
Berlingen	2180.64	Saddle dolomite	Pore-filling	TD	13.8	>138–142	-1.6 to -1.3
Berlingen	2189.45	Saddle dolomite	Pore-filling	TD	13.5	>138–142	-2.0 to -1.6
Berlingen	2181.37	Saddle dolomite	Pore-filling	TD	15.0	>138–142	-0.4 to -0.1
Berlingen	2189.11	Saddle dolomite	Pore-filling	TD	14.6	>138–142*	-0.9 to -0.5
Siblingen	1023.62	Calcite	Fracture-filling	CB	11.9	65–75*	-9.5 to -8.2
Siblingen	770.36	Calcite	Fracture-filling	CB	11.5 ¹	65–75	-9.9 to -8.5
Siblingen	1162.67	Calcite	Fracture-filling	CB	12.5 ¹	65–75	-9.0 to -7.6
Siblingen	1249.04	Calcite	Fracture-filling	CB	12.0 ¹	65–75	-9.4 to -8.1
Siblingen	1371.68	Calcite	Fracture-filling	CB	10.7 ¹	65–75	-10.7 to -9.3
Leuggern	318.65	Calcite	Fracture-filling	CB	20.8	85–95*	2.0 to 3.2
Leuggern	863.35	Calcite	Fracture-filling	CB	12.4 ²	65–75	-9.1 to -7.7
Leuggern	949.88	Calcite	Fracture-filling	CB	14.1 ²	65–75	-7.3 to -5.9
Leuggern	1046.05	Calcite	Fracture-filling	CB	11.3 ²	65–75	-10.2 to -8.8
Leuggern	1188.00	Calcite	Fracture-filling	CB	12.5 ²	65–75	-8.9 to -7.5
Leuggern	1197.42	Calcite	Fracture-filling	CB	11.9 ²	65–75	-9.5 to -8.2
Leuggern	1212.7	Calcite	Fracture-filling	CB	11.2 ²	65–75	-10.2 to -8.9
Leuggern	1298.18	Calcite	Fracture-filling	CB	10.8 ²	65–75	-10.7 to -9.3
Kaisten	799.88	Calcite	Fracture-filling	CB	14.2 ³	65–75	-7.3 to -5.9
Kaisten	819.67	Calcite	Fracture-filling	CB	14.4 ³	65–75	-7.0 to -5.7
Kaisten	834.28	Calcite	Fracture-filling	CB	13.7 ³	65–75	-7.8 to -6.4
Kaisten	846.88	Calcite	Fracture-filling	CB	15.0 ³	65–75	-6.4 to -5.0
Kaisten	918.72	Calcite	Fracture-filling	CB	13.0 ³	65–75	-8.5 to -7.1
Kaisten	1048.8	Calcite	Fracture-filling	CB	14.6 ³	65–75	-6.8 to -5.5
Kaisten	1205.11	Calcite	Fracture-filling	CB	11.7 ³	65–75	-9.7 to -8.3
Kaisten	1273.94	Calcite	Fracture-filling	CB	14.5 ³	65–75	-6.9 to -5.6
Kaisten	1273.94	Calcite	Fracture-filling	CB	10.8 ³	65–75	-10.6 to -9.3

TD: Trigonodus Dolomit

HMK: Hauptmuschelkalk

DAG: Dolomit der Anhydritgruppe

CB: Crystalline basement

 T_{trap} : Fluid inclusion trapping temperature

*: Samples with constraints on precipitation temperature from fluid inclusion studies.

Those temperatures provide the basis for calculating the parent-water of samples without temperature constraints from fluid inclusion studies.

¹ Nagra [51]² Peters et al. [47]³ Nagra [50]

A5

Table A.5: Results of the oxygen and hydrogen isotope analyses of secondary kaolinite and calculated parent-waters from various wells across the Swiss Molasse Basin.

Well	Sample depth (m)	Phase	Occurrence	Unit	$\delta^{18}\text{O}_{\text{mineral}}$ (‰ VSMOW)	$\delta^2\text{H}_{\text{mineral}}$ (‰ VSMOW)	$T_{\text{precip.}}$ (° C)	$\delta^{18}\text{O}_{\text{parent-water}}$ (‰ VSMOW)	$\delta^2\text{H}_{\text{parent-water}}$ (‰ VSMOW)
Benken	811.36	Kaolinite	Pore-filling	TD	10.00	-82.0	85–88	-4.77 to -4.41	-57.4 to -57.2
Benken	833.87	Kaolinite	Pore-filling	TD	9.80	-80.5	85–88	-4.97 to -4.61	-55.9 to -55.7
Benken	839.81	Kaolinite	Pore-filling	TD	9.30	-80.2	85–88	-5.47 to -5.11	-55.6 to -55.4
Benken	839.81	Kaolinite	Pore-filling	TD	10.19	-78.5	85–88	-4.58 to -4.22	-53.9 to -53.7
Benken	811.36	Kaolinite	Pore-filling	TD	10.23	-79.9	85–88	-4.54 to -4.18	-55.3 to -55.1
Benken	826.87	Kaolinite	Pore-filling	TD	10.61	-87.5	85–88	-4.16 to -3.8	-62.9 to -62.7
Schlattingen	1130.94	Kaolinite	Pore-filling	TD	9.36	-82.0	76–89	-6.53 to -4.93	-56.5 to -57.3
Schlattingen	1127.44	Kaolinite	Pore-filling	TD	9.17	-85.5	76–89	-6.72 to -5.12	-61.0 to -59.8
Schlattingen	1130.50	Kaolinite	Pore-filling	TD	8.28	-88.5	76–89	-7.61 to -6.01	-64.0 to -62.8
Weiach	843.36	Kaolinite	Pore-filling	TD	10.90	-86.5	76–89	-4.99 to -3.39	-62.0 to -60.8
Schlattingen	1159.50	Kaolinite	Pore-filling	HMK	10.14	-83.0	76–89	-5.75 to -4.15	-58.5 to -57.3
Schlattingen	1164.33	Kaolinite	Pore-filling	HMK	9.46	-91.0	76–89	-6.43 to -4.83	-66.5 to -65.3
Siblingen	401.82	Kaolinite	Fracture-filling	CB		-91.9	70–80		-66.5 to -65.5
Siblingen	456.34	Kaolinite	Fracture-filling	CB		-94.1	71–81		-69.5 to -68.6
Siblingen	659.67	Kaolinite	Fracture-filling	CB		-95.6	78–88		-71.1 to -70.1
Siblingen	701.29	Kaolinite	Fracture-filling	CB		-91.5	79–89		-67.0 to -66.0
Siblingen	828.11	Kaolinite	Fracture-filling	CB		-91.4	83–93		-67.3 to -66.3
Siblingen	915.58	Kaolinite	Fracture-filling	CB		-90.3	85–95		-66.1 to -65.2
Siblingen	922.95	Kaolinite	Fracture-filling	CB		-89.3	85–95		-65.4 to -64.4

TD: Trigonodus Dolomit

HMK: Hauptmuschelkalk

CB: Crystalline basement

$T_{\text{precip.}}$: Precipitation temperature of kaolinite derived from
fluid inclusion studies in coeval calcite

A6

Table A.6: Results of the sulphur isotope analyses of anhydrite nodules and secondary pore- and fracture-filling anhydrite in the Muschelkalk and the overlying Keuper.

Well	Sample depth (m)	Mineral	Occurrence	Unit	$\delta^{34}\text{S}_{\text{anhydrite}}$ (‰ VCDT)
Benken	931.75 M	Anhydrite	Rock	Sulfatschichten	18.8 ¹
Weiach	910.15	Anhydrite	Massive bed	Sulfatschichten	18.5 ²
Böttstein	241.16	Anhydrite	Rock	Sulfatschichten	19.5 ²
Schafisheim	1294.17	Anhydrite	Massive bed	DAG	18.6
Schafisheim	1295.76	Anhydrite	Massive bed	DAG	18.5
Weiach	824.85	Anhydrite	Blocky anhydrite, nodule	TD	19.2 ²
Weiach	828.72	Anhydrite	Felted anhydrite, nodule	TD	18.7 ²
Schlattingen	1121.87	Anhydrite	Nodule	TD	19.9
Schlattingen	1133.43	Anhydrite	Nodule	TD	19.8
Schafisheim	1234.67	Anhydrite	Massive bed	TD	18.0
Benken	748.18	Anhydrite	Nodule	Gipskeuper	12.5 ¹
Benken	766.51	Anhydrite	Bed	Gipskeuper	13.8 ¹
Böttstein	59.37	Gypsum	Nodule	Gipskeuper	14.3 ²
Böttstein	59.00	Gypsum	Satin spar	Gipskeuper	14.0 ²
Böttstein	80.00	Gypsum	Satin spar	Gipskeuper	14.0 ²
Böttstein	88.90	Anhydrite	Pseudom. after satin spar	Gipskeuper	15.0 ²
Böttstein	115.50	Gypsum	Interlayered with dolomite	Gipskeuper	15.9 ²
Schafisheim	1189.60	Anhydrite	Bed	Gipskeuper	14.4
Schafisheim	1207.30	Anhydrite	Bed	Gipskeuper	14.9
Schafisheim	1334.99	Anhydrite	Fracture-filling	HMK	18.9
Schafisheim	1329.20	Anhydrite	Fracture-filling	HMK	17.7 ²
Böttstein	158.23	Anhydrite	Pore-filling	HMK	19.8 ²
Schlattingen	1116.66	Anhydrite	Fracture-filling	TD	18.8
Schlattingen	1135.58	Anhydrite	Pore-filling	TD	20.2
Schlattingen	1136.98	Anhydrite	Pore-filling	TD	20.4
Schlattingen	1135.29	Anhydrite	Pore-filling	TD	17.5
Schlattingen	1140.15	Anhydrite	Pore-filling	TD	17.3
Schafisheim	1231.47	Anhydrite	Pore-filling	TD	17.8
Schafisheim	1234.38	Anhydrite	Pore-filling	TD	17.6
Schafisheim	1228.45	Anhydrite	Fracture-filling	TD	18.3
Schafisheim	1230.09	Anhydrite	Pore-filling	TD	17.3
Berlingen	2184.87	Anhydrite	Fracture-filling	TD	17.8
Berlingen	2182.08	Anhydrite	Fracture-filling	TD	18.6
Schlattingen	1116.66	Anhydrite	Fracture-filling	TD	19.5
Schlattingen	1136.98	Anhydrite	Pore-filling	TD	19.2
Benken	771.51	Anhydrite	Fracture-filling	Keuper	14.4 ¹
Benken	730.76	Anhydrite	Fracture-filling	Keuper	13.5 ¹

TD: Trigonodus Dolomit

HMK: Hauptmuschelkalk

DAG: Dolomit der Anhydritgruppe

¹ Nagra [38]

² Pearson et al. [20]

A7

Table A.7: Results of the LA-ICP-MS analyses of secondary calcites from the wells at Benken, Schlattingen, Siblingen and Leuggern.

Sample/ Spot	U (ppm)	²⁰⁶ Pb (ppm)	Th/U	²⁰⁷ Pb/ ²³⁵ U	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ	Err. correl.	Model age (Ma)	1σ	²⁰⁷ Pb/ ²³⁵ U Age (Ma)	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ
BEN839.81														
NIST612 - 213 nm														
BEN839-1	0.061	.	0.1	0.150235	0.088	0.00534	0.0011	0.36702	27	8	34	7	142	75
BEN839-2	0.274	0.002	0.11	0.598128	0.092	0.00548	0.0005	0.54445	2	4	35	3	476	57
BEN839-12	0.758	0.007	0.02	0.610677	0.043	0.00865	0.0003	0.49423	23	2	56	2	484	27
BEN839-3	0.215	0.002	0.13	0.82216	0.106	0.01002	0.0007	0.51546	19	6	64	4	609	58
BEN839-14	0.656	0.009	0.02	1.286619	0.071	0.01305	0.0004	0.54032	12	4	84	2	840	31
BEN839-23	0.702	0.009	0.04	1.277292	0.089	0.0133	0.0005	0.53919	15	4	85	3	836	39
BEN839-8	0.385	0.005	0.03	1.383389	0.099	0.01422	0.0006	0.54044	15	5	91	4	882	42
BEN839-13	0.617	0.01	0.02	1.670032	0.087	0.01622	0.0005	0.54882	11	4	104	3	997	33
BEN839-15	0.639	0.01	0.02	1.640584	0.081	0.0164	0.0004	0.54564	14	4	105	3	986	31
BEN839-18	0.696	0.013	0.02	1.651514	0.076	0.0186	0.0005	0.53468	28	4	119	3	990	29
BEN839-21	0.447	0.009	0.03	1.918666	0.129	0.01944	0.0007	0.54913	18	6	124	5	1088	44
BEN839-5	0.072	0.002	0.03	2.423535	0.31	0.02563	0.0018	0.54882	30	16	163	11	1250	89
BEN839-22	0.679	0.018	0.02	2.775678	0.111	0.02648	0.0006	0.56348	15	5	168	4	1349	30
BEN839-16	0.434	0.015	0.03	3.494894	0.24	0.03506	0.0014	0.5638	31	12	222	8	1526	53
BEN839-19	0.668	0.025	0.02	4.106037	0.141	0.03806	0.0008	0.57753	15	7	241	5	1656	28
BEN839-10	0.836	0.039	0.04	4.932833	0.132	0.04634	0.0007	0.58373	22	6	292	4	1808	22
BEN839-4	0.178	0.009	0.1	5.811576	0.356	0.05301	0.0019	0.59152	15	17	333	12	1948	52
BEN839-9	0.715	0.045	0.02	7.09993	0.161	0.06263	0.0009	0.6049	4	7	392	5	2124	20
BEN839-24	0.556	0.035	0.03	6.777602	0.199	0.06264	0.0011	0.60059	23	9	392	7	2083	26
BEN839-17	0.484	0.047	0.02	10.80853	0.276	0.09673	0.0016	0.62907	16	13	595	9	2507	24
BEN839-20	0.671	0.08	0.02	12.94146	0.267	0.11919	0.0016	0.64303	42	12	726	9	2675	19
BEN839-11	0.53	0.082	0.08	17.25825	0.445	0.15401	0.0026	0.6664	22	20	923	15	2949	25
BEN839-7	0.405	0.081	0.02	22.75651	0.5	0.20003	0.003	0.69217	8	20	1175	16	3217	21
BEN839-6	0.165	0.09	0.03	61.4615	1.368	0.54715	0.0097	0.79866	69	49	2813	40	4198	22

Continuation of Table A.7

Sample/ Spot	U (ppm)	²⁰⁶ Pb (ppm)	Th/U	²⁰⁷ Pb/ ²³⁵ U	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ	Err. correl.	Model age (Ma)	1σ	²⁰⁷ Pb/ ²³⁵ U Age (Ma)	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ
BEN840.10														
NIST612 - 213 nm														
BEN840-10	0.618	0.005	0.06	0.577	0.050	0.0084	0.0004	0.4907	23	3	54	2	462	32
BEN840-9.2	0.136	0.001	0.10	0.641	0.047	0.0085	0.0003	0.5033	20	3	55	2	503	29
BEN840-11.2	0.179	0.002	0.07	0.753	0.047	0.0085	0.0003	0.5237	13	2	54	2	570	27
BEN840-10.2	0.122	0.001	0.07	0.950	0.057	0.0108	0.0003	0.5251	17	3	69	2	678	29
BEN840-11.3	0.121	0.001	0.07	0.991	0.059	0.0106	0.0003	0.5326	13	3	68	2	699	30
BEN840-11.4	0.185	0.002	0.13	1.140	0.062	0.0123	0.0004	0.5333	16	3	79	2	773	29
BEN840-10.5	0.13	0.002	0.06	1.227	0.066	0.0123	0.0004	0.5423	10	3	79	2	813	30
BEN840-11	0.701	0.010	0.07	1.412	0.078	0.0145	0.0004	0.5404	15	4	93	3	894	32
BEN840-10.3	0.116	0.002	0.07	1.851	0.093	0.0189	0.0005	0.5470	18	5	121	3	1064	33
BEN840-9	0.508	0.012	0.13	2.301	0.114	0.0233	0.0006	0.5507	22	6	149	4	1213	35
BEN840-12	0.514	0.012	0.02	2.555	0.143	0.0243	0.0008	0.5596	14	7	155	5	1288	40
BEN840-11.5	0.131	0.004	0.04	2.643	0.102	0.0271	0.0006	0.5554	27	5	172	4	1313	28
BEN840-10.4	0.137	0.004	0.05	2.664	0.100	0.0262	0.0005	0.5588	20	5	167	3	1319	27
BEN840-9.3	0.074	0.002	0.13	3.200	0.166	0.0319	0.0009	0.5626	27	8	202	6	1457	39
BEN840-6	0.055	0.002	0.04	4.358	0.596	0.0410	0.0032	0.5754	20	28	259	20	1704	109
BEN840-7	0.205	0.009	0.02	4.644	0.306	0.0423	0.0016	0.5803	12	14	267	10	1757	54
BEN840-4	0.174	0.010	0.02	6.689	0.353	0.0600	0.0019	0.5965	11	16	376	11	2071	46
BEN840-8	0.785	0.087	0.01	12.664	0.257	0.1105	0.0014	0.6379	-1	10	675	8	2655	19
BEN840-5	0.354	0.046	0.04	14.028	0.353	0.1308	0.0021	0.6429	56	16	793	12	2752	24
BEN853.92														
NIST612 - 193 nm														
BEN853.82-12-24	2.136	0.004	0.06	0.019	0.006	0.0019	0.0001	0.2108	12	1	12	1	19	6
BEN853.82-12-26	2.208	0.005	0.07	0.023	0.007	0.0021	0.0001	0.2201	13	1	13	1	23	7
BEN853.82-12-23	1.648	0.004	0.06	0.024	0.008	0.0022	0.0002	0.2173	14	1	14	1	24	8
BEN853.82-12-20	1.941	0.004	0.06	0.030	0.009	0.0018	0.0001	0.2619	11	1	12	1	30	9

Continuation of Table A.7

Sample/ Spot	U (ppm)	²⁰⁶ Pb (ppm)	Th/U	²⁰⁷ Pb/ ²³⁵ U	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ	Err. correl.	Model age (Ma)	1σ	²⁰⁷ Pb/ ²³⁵ U Age (Ma)	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ
BEN853.82-12-21	2.649	0.005	0.06	0.033	0.008	0.0019	0.0001	0.2697	11	1	12	1	33	8
BEN853.82-12-28	1.518	0.003	0.07	0.037	0.011	0.0019	0.0002	0.2796	11	1	12	1	36	11
BEN853.82-12-30	2.021	0.005	0.07	0.036	0.009	0.0022	0.0001	0.2588	13	1	14	1	36	9
BEN853.82-12-19	1.726	0.004	0.06	0.041	0.011	0.0021	0.0002	0.2806	12	1	14	1	40	11
BEN853.82-12-22	2.054	0.004	0.06	0.040	0.010	0.0019	0.0001	0.2886	11	1	12	1	40	9
BEN853.82-12-13	1.644	0.003	0.06	0.045	0.013	0.0019	0.0002	0.3060	10	1	12	1	45	12
BEN853.82-12-5	1.963	0.004	0.07	0.046	0.011	0.0021	0.0001	0.2948	12	1	14	1	46	11
BEN853.82-12-4	1.324	0.003	0.07	0.049	0.014	0.0022	0.0002	0.2990	12	1	14	1	49	14
BEN853.82-12-25	1.8	0.004	0.07	0.054	0.012	0.0025	0.0002	0.2962	14	1	16	1	53	12
BEN853.82-12-14	1.069	0.003	0.07	0.058	0.018	0.0026	0.0002	0.3001	14	2	16	2	57	17
BEN853.82-12-15	1.534	0.003	0.06	0.062	0.014	0.0021	0.0002	0.3333	11	1	14	1	61	14
BEN853.82-12-29	1.703	0.003	0.07	0.063	0.015	0.0019	0.0002	0.3518	9	1	12	1	62	15
BEN853.82-12-1	1.669	0.004	0.07	0.073	0.015	0.0022	0.0002	0.3483	11	1	14	1	71	14
BEN853.82-12-16	1.567	0.004	0.06	0.087	0.017	0.0026	0.0002	0.3511	12	1	17	1	85	16
BEN853.82-12-17	1.201	0.003	0.07	0.090	0.021	0.0022	0.0002	0.3772	10	1	14	1	88	19
BEN853.82-12-27	0.764	0.002	0.07	0.125	0.033	0.0026	0.0003	0.4013	10	2	16	2	119	29
BEN853.82-12-3	0.985	0.004	0.18	0.177	0.047	0.0036	0.0004	0.4040	14	3	23	2	166	40
BEN853.82-12-18	1.155	0.004	0.10	0.239	0.044	0.0033	0.0003	0.4532	9	2	21	2	218	36
BEN853.82-12-8	2.172	0.035	0.14	1.602	0.094	0.0159	0.0005	0.5029	13	5	102	3	971	36
BEN853.82-12-2	2.094	0.130	0.10	6.704	0.193	0.0621	0.0009	0.5290	24	10	388	6	2073	25
BEN853.82-12-6	1.731	0.114	0.08	7.273	0.194	0.0660	0.0009	0.5331	17	10	412	6	2145	24
LEU54.78														
NIST612 - 213 nm														
LEU54_78-13.5	3.454	0.012	0.00	0.156	0.011	0.0035	0.0001	0.4315	14	1	22	1	147	10
LEU54_78-3.2	2.277	0.008	0.00	0.162	0.009	0.0034	0.0001	0.4376	14	1	22	1	153	8
LEU54_78-13.1	5.488	0.023	0.00	0.256	0.010	0.0041	0.0001	0.4761	13	1	26	0	231	8
LEU54_78-3.1	3.679	0.017	0.00	0.319	0.012	0.0045	0.0001	0.4925	12	1	29	1	281	10

Continuation of Table A.7

Sample/ Spot	U (ppm)	²⁰⁶ Pb (ppm)	Th/U	²⁰⁷ Pb/ ²³⁵ U	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ	Err. correl.	Model age (Ma)	1σ	²⁰⁷ Pb/ ²³⁵ U Age (Ma)	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ
LEU54_78-3.9	2.135	0.012	0.00	0.370	0.018	0.0055	0.0001	0.4871	16	1	36	1	320	13
LEU54_78-3.8	3.228	0.018	0.00	0.408	0.013	0.0056	0.0001	0.4992	14	1	36	1	347	9
LEU54_78-13.2	2.459	0.015	0.00	0.439	0.021	0.0060	0.0001	0.4984	15	1	39	1	370	15
LEU54_78-3.7	2.384	0.016	0.00	0.543	0.019	0.0065	0.0001	0.5165	12	1	42	1	441	13
LEU54_78-13.4	4.114	0.029	0.00	0.548	0.016	0.0071	0.0001	0.5083	15	1	45	1	443	10
LEU54_78-13.3	5.076	0.037	0.00	0.586	0.015	0.0073	0.0001	0.5135	15	1	47	1	468	9
LEU54_78-3.3	3.176	0.035	0.00	1.023	0.024	0.0109	0.0001	0.5362	13	1	70	1	716	12
LEU54_78-13.12	0.449	0.007	0.00	1.510	0.118	0.0147	0.0006	0.5500	10	6	94	4	935	47
SIB241.60														
NIST612 - 213 nm														
SIB241-9	3.161	0.010	0.01	0.075655	0.008	0.0031	0.0001	0.3465	17	1	20	1	74	7
SIB241-10	3.743	0.012	0.01	0.083846	0.007	0.0032	0.0001	0.3579	17	1	20	1	82	7
SIB241-10.4	3.845	0.012	0.02	0.08878	0.005	0.0032	0.0001	0.3639	16	0	21	0	86	5
SIB241-10.6	5.976	0.019	0.01	0.092028	0.004	0.0032	0.0000	0.3675	17	0	21	0	89	3
SIB241-10.5.3	4.342	0.020	0.02	0.216338	0.008	0.0046	0.0001	0.4384	18	1	29	0	199	7
SIB241-10.5.2	1.474	0.008	0.02	0.252873	0.013	0.0053	0.0001	0.4399	21	1	34	1	229	11
SIB241-10.5.4	0.867	0.005	0.04	0.305951	0.021	0.0061	0.0002	0.4477	23	1	39	1	271	16
SIB241-8	1.022	0.006	0.03	0.443213	0.03	0.0063	0.0002	0.4929	16	2	40	1	373	21
SIB241-10.3	0.832	0.005	0.03	0.401069	0.028	0.0065	0.0002	0.4759	20	2	42	1	342	20
SIB241-6	0.496	0.003	0.03	0.439921	0.045	0.0067	0.0003	0.4833	20	3	43	2	370	31
SIB241-2	0.548	0.005	0.09	0.605894	0.058	0.0088	0.0004	0.4918	24	3	56	3	481	36
SIB241-10.5	0.984	0.013	0.04	1.023652	0.042	0.0130	0.0003	0.5137	28	2	83	2	716	21
SIB241-5	0.415	0.007	0.04	1.332638	0.164	0.0170	0.0011	0.5165	36	9	109	7	860	70
SIB241-10.2	0.523	0.010	0.03	1.66538	0.068	0.0198	0.0004	0.5289	36	4	126	3	995	26
SIB241-3	0.595	0.017	0.16	2.691173	0.115	0.0287	0.0007	0.5491	36	6	183	4	1326	31

Continuation of Table A.7

Sample/ Spot	U (ppm)	²⁰⁶ Pb (ppm)	Th/U	²⁰⁷ Pb/ ²³⁵ U	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ	Err. correl.	Model age (Ma)	1σ	²⁰⁷ Pb/ ²³⁵ U Age (Ma)	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ
SIB630.02														
NIST612 - 213 nm														
SIB630-11	22.82	1.168	0.80	5.342254	0.021	0.0512	0.0001	0.6008	31	1	322	1	1876	3
SIB630-13	43.45	2.329	0.59	5.551641	0.031	0.0536	0.0002	0.5952	35	1	337	1	1909	5
SIB630-5.3	6.71	0.423	0.05	6.563168	0.062	0.0630	0.0004	0.5998	38	3	394	2	2054	8
SIB630-15	14.67	1.216	0.50	8.603445	0.057	0.0829	0.0003	0.6182	53	3	514	2	2297	6
SIB630-12	17.56	1.467	0.17	8.859905	0.054	0.0835	0.0003	0.6201	41	2	517	2	2324	6
SIB630-5	19.36	1.688	0.02	9.128006	0.042	0.0872	0.0003	0.6269	51	2	539	2	2351	4
SIB630-5.2	22.60	2.143	0.02	9.922489	0.041	0.0948	0.0002	0.6318	55	2	584	1	2428	4
SIB630-14.2	20.34	2.210	0.12	11.74599	0.07	0.1086	0.0004	0.6408	41	3	665	2	2584	6
SIB630-15.2	2.33	0.679	0.55	31.69403	0.289	0.2918	0.0019	0.7323	101	12	1651	10	3541	9
SIB630-14	11.15	3.297	0.26	32.04601	0.101	0.2957	0.0007	0.7298	107	4	1670	3	3552	3
SIB630-11.2	2.91	1.049	0.54	38.00044	0.198	0.3608	0.0014	0.7502	194	8	1986	7	3720	5
SIB630-13.2	6.47	2.439	0.56	40.00204	0.195	0.3771	0.0014	0.7562	186	7	2063	6	3771	5
SIB630-12.2	3.84	1.639	0.35	46.12041	0.272	0.4272	0.0019	0.7712	164	10	2293	9	3912	6
SIB1023.62														
NIST612 - 213 nm														
SIB1023-3.4	26.48	0.112	0.02	0.342512	0.004	0.0042	0.0000	0.5110	8	0	27	0	299	3
SIB1023-7.6	23.55	0.117	0.02	0.425782	0.006	0.0050	0.0000	0.5190	9	0	32	0	360	4
SIB1023-7.1	10.82	0.079	0.03	0.690189	0.012	0.0073	0.0001	0.5320	8	1	47	0	533	7
SIB1023-7.5	11.61	0.102	0.02	0.853614	0.011	0.0088	0.0001	0.5376	9	1	57	0	627	6
SIB1023-3.1	16.51	0.183	0.02	1.100802	0.014	0.0111	0.0001	0.5424	10	1	71	0	754	7
SIB1023-7.3	6.36	0.077	0.03	1.255945	0.022	0.0121	0.0001	0.5470	8	1	78	1	826	10
SIB1023-3.2	9.38	0.129	0.03	1.422853	0.028	0.0137	0.0001	0.5483	9	1	88	1	899	12
SIB1023-7.2	5.19	0.087	0.07	1.772464	0.027	0.0168	0.0001	0.5538	9	1	108	1	1035	10
SIB1023-7.9	3.15	0.084	0.08	2.886046	0.048	0.0266	0.0003	0.5677	9	2	169	2	1378	13
SIB1023-7.8	9.92	0.266	0.02	2.919298	0.025	0.0268	0.0001	0.5706	9	1	171	1	1387	7

Continuation of Table A.7

Sample/ Spot	U (ppm)	²⁰⁶ Pb (ppm)	Th/U	²⁰⁷ Pb/ ²³⁵ U	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ	Err. correl.	Model age (Ma)	1σ	²⁰⁷ Pb/ ²³⁵ U Age (Ma)	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ
SIB1023-7.4	12.00	0.381	0.03	3.470085	0.025	0.0317	0.0001	0.5766	10	1	201	1	1520	6
SIB1023-7.7	15.47	0.723	0.01	5.178799	0.027	0.0468	0.0001	0.5955	10	1	295	1	1849	4
SIB1023-3.3	6.14	0.293	0.04	5.270473	0.044	0.0477	0.0002	0.5895	11	2	300	1	1864	7
SLA1167.68														
NIST612 - 213 nm														
SLA1167.88-17	3.21	0.013	0.02	0.211021	0.042	0.0041	0.0003	0.4072	16	3	27	2	194	34
SLA1167.88-27	0.68	0.003	0.02	0.378038	0.073	0.0048	0.0004	0.4678	10	4	31	3	326	53
SLA1167.88-21	16.43	0.110	0.00	0.507156	0.015	0.0067	0.0001	0.4637	15	1	43	1	417	10
SLA1167.88-11	1.13	0.008	0.02	0.634542	0.103	0.0073	0.0006	0.4795	12	5	47	4	499	63
SLA1167.88-19	24.58	0.204	0.00	0.674926	0.014	0.0083	0.0001	0.4743	16	1	53	1	524	9
SLA1167.88-28	0.44	0.004	0.02	0.561043	0.189	0.0092	0.0014	0.4341	30	11	59	9	452	118
SLA1167.88-20	27.53	0.262	0.00	0.813315	0.016	0.0095	0.0001	0.4809	16	1	61	1	604	9
SLA1167.88-10	1.12	0.011	0.03	0.88036	0.096	0.0102	0.0005	0.4805	17	5	65	3	641	51
SLA1167.88-14	23.34	0.267	0.00	1.048773	0.019	0.0115	0.0001	0.4900	16	1	73	1	728	9
SLA1167.88-9	1.67	0.020	0.04	1.034136	0.133	0.0123	0.0008	0.4781	22	7	79	5	721	65
SLA1167.88-26	0.69	0.009	0.03	1.236749	0.14	0.0123	0.0007	0.5013	10	7	79	4	817	62
SLA1167.88-22	1.93	0.028	0.02	1.366415	0.08	0.0143	0.0004	0.4958	16	4	92	3	875	34
SLA1167.88-24	8.46	0.134	0.01	1.524356	0.037	0.0159	0.0002	0.4983	17	2	102	1	940	15
SLA1167.88-1	1.41	0.028	0.02	2.01848	0.121	0.0198	0.0006	0.5060	15	6	127	4	1122	40
SLA1167.88-23	1.38	0.028	0.02	1.817404	0.12	0.0203	0.0007	0.4903	30	6	129	4	1052	43
SLA1167.88-4	10.76	0.256	0.00	2.389494	0.061	0.0238	0.0003	0.5062	20	3	152	2	1239	18
SLA1167.88-15	30.01	0.749	0.00	2.534718	0.027	0.0249	0.0001	0.5106	19	1	159	1	1282	8
SLA1167.88-13	15.49	0.425	0.00	2.81209	0.042	0.0274	0.0002	0.5116	19	2	174	1	1359	11
SLA1167.88-25	3.26	0.101	0.02	3.28592	0.113	0.0309	0.0005	0.5163	15	6	196	3	1478	27
SLA1167.88-7	16.66	0.548	0.00	3.426384	0.041	0.0329	0.0002	0.5174	20	2	209	1	1510	9
SLA1167.88-12	2.08	0.075	0.01	3.666293	0.235	0.0359	0.0012	0.5119	26	12	227	7	1564	50
SLA1167.88-8	5.35	0.203	0.02	3.898581	0.098	0.0379	0.0005	0.5145	26	5	240	3	1613	20

Continuation of Table A.7

Sample/ Spot	U (ppm)	²⁰⁶ Pb (ppm)	Th/U	²⁰⁷ Pb/ ²³⁵ U	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ	Err. correl.	Model age (Ma)	1σ	²⁰⁷ Pb/ ²³⁵ U Age (Ma)	1σ	²⁰⁶ Pb/ ²³⁸ U	1σ
SLA1167.88-6	4.03	0.163	0.02	4.237806	0.104	0.0403	0.0005	0.5187	22	5	255	3	1681	20
SLA1167.88-18	4.80	0.234	0.01	5.069222	0.124	0.0487	0.0006	0.5202	30	6	307	4	1831	21
SLA1167.88-16	6.13	0.645	0.01	11.14024	0.178	0.1053	0.0009	0.5422	54	9	646	5	2535	15

A8

As a consistency test for the favoured scenario in which saline brine in the Muschelkalk dolostones mixes with a dilute fluid ascending from the basement, a simple thermodynamic model has been constructed using the software *PhreeqC* [62]. The brine (composition defined in Table A.8) was assumed to be in equilibrium with dolomite and anhydrite at 50 °C, whereas the dilute fluid (composition of a recent groundwater from the crystalline basement in Wittwer [61]; Table A.8) was assumed to be in equilibrium with calcite but undersaturated with respect to anhydrite at 65 °C.

The results show that mixing will spontaneously result in dissolution of anhydrite (saturation index, $S.I. < 0$ in Fig. A.8) and precipitation of secondary calcite and dolomite ($S.I. > 0$ in Fig. A.8) over a wide range of volumetric mixing ratios (supersaturation of dolomite is mainly caused by the large contrast in the calcium and magnesium concentrations of the endmembers). The model is therefore broadly consistent with the observations. However, as both carbonate minerals are supersaturated in this model, it is not clear why calcite precipitates alone in the shallow wells, whereas dolomite precipitates alone in the deep wells. Quartz and kaolinite precipitation on the other hand is probably triggered by cooling of the silica- and alumina-bearing basement water upon its ascent or upon mixing with the colder brine in the dolostones.

Table A.8: Chemical data on evaporative brine [57] and basement water from the Weiach well [61].

Parameter	Brine	Basement water
pH	6.6	7.66
Temperature (°C)	50	65
Pressure (MPa)	12	19
Na ⁺ (mg/L)	82120	2205
K ⁺ (mg/L)	4240	70.4
Mg ²⁺ (mg/L)	10000	0.1
Ca ²⁺ (mg/L)	11250	152
Cl ⁻ (mg/L)	176350	3382
SO ₄ ²⁻ (mg/L)	3920	431
Alkalinity (mg/L)	56	76

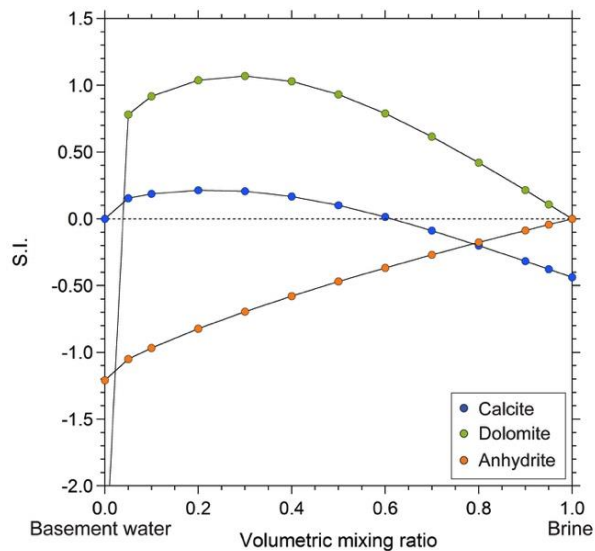


Fig. A.8. Saturation indices (*S.I.*) of calcite, dolomite and anhydrite as a function of the volumetric mixing ratio between a hypersaline brine at 50 °C (residual Triassic dolomitizing pore water) and a recent groundwater from the crystalline basement at 65 °C, calculated using PhreeqC and data in Table A.8.

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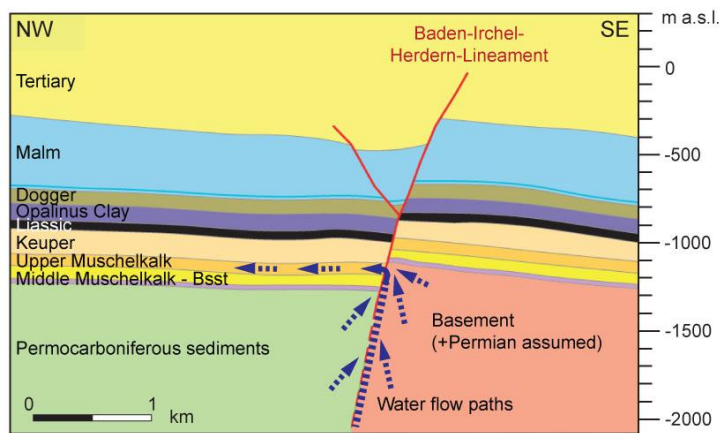


Fig. A.9. Deduced infiltration of basement fluid on an interpreted NW–SE seismic transect of the Baden–Irchel–Herdern Lineament, at the margin of a Permo-carboniferous through. The fault has a throw of about 150 m, which juxtaposes the basement and the Upper Muschelkalk. Thus, ascending basement water can bypass the Middle Muschelkalk Sulfatschichten and directly infiltrate the Upper Muschelkalk (Bsst: Buntsandstein; see Fig. 1a to locate the profile; modified after Nagra, 2014).

References:

- Nagra (2014) SGT Etappe 2: Vorschlag weiter zu untersuchender geologischer Standortgebiete mit zugehörigen Standortarealen für die Oberflächenanlage – Geologische Grundlagen Dossier II; Sedimentologische und tektonische Verhältnisse. Nagra Technischer Bericht NTB 14-02. Nagra, Wettingen, Switzerland.