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Experimental Work Conducted on MgO Long-Term Hydration

2008 Milestone Report

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1 INTRODUCTION

Magnesium oxide (MgO) is being emplaced in the WIPP as an engineered barrier to sequester carbon dioxide (CO_2) that could potentially be generated by microbial consumption of the cellulose, plastic and rubber in the repository. MgO also consumes water in brine or water vapor in the gas phase to form brucite, $Mg(OH)_2$. The brucite dissolution reaction will buffer pH to a slightly alkaline pH (U.S. DOE, 2004), which directly affects actinide speciation and solubility. The strong reducing conditions created by anoxic iron corrosion, low f_{CO_2} and the mildly basic brine will result in low actinide (An) solubility.

A series of experiments have been conducted at SNL to verify the efficacy of MgO from Martin Marietta Magnesia Specialties LLC (Martin Marietta) under test plan TP 06-03. There are three tasks in TP 06-03: MgO characterization, MgO hydration, and MgO carbonation. MgO characterization, accelerated MgO hydration under inundated conditions were completed and reported in the last milestone report (Deng et al., 2008). Currently three experiments are being carried out: humid hydration, long-term inundated hydration, and MgO carbonation. Only the long-term inundated hydration data will be discussed in this report. The other two sets of experiments will be reported at a later time when more data is collected.

Particle size, solid-to-liquid ratio, and stir speed may all influence MgO hydration kinetics. Accelerated-MgO-hydration experiments were carried out with two MgO particle sizes, three solid-to-liquid ratios and two stir speeds in de-ionized (DI) water at 70 ºC (Deng et al., 2008). We found that the MgO particle size is the most important factor affecting the hydration rate while the solid-to-liquid ratio, and stir speed do not have a significant effect on the hydration rate. Based on these results, we designed a long-term-MgO-hydration experimental matrix where the effect of the MgO particle size would be carefully tested. The fractional-factorial (Box et al., 1978) experimental matrix was designed to test the hydration rate with three MgO particle sizes and two solid-to-liquid ratios in three WIPP-related brines. EQ3/6 was used to simulate the reaction path way of MgO hydration and carbonation in a closed system containing brine and atmospheric carbon dioxide by titrating periclase into the system. This activity is covered by analysis plan AP-108 (Nowak, 2003). This work is a deviation from that analysis plan where no EQ3/6 or FMT runs were originally planned. Experimentally measured pH, Mg^{2+}, and Cl^- concentration, and the phase assemblage of hydration products are compared with the modeling predictions.

2 DESCRIPTION OF THE LONG-TERM INUNDATED HYDRATION EXPERIMENTS

2.1 Experiment matrix

A fractional-factorial (Box et al., 1978) experimental matrix was designed to test the hydration rate with three MgO particle sizes and two solid-to-liquid ratios in three WIPP-related brines. MgO sieved into three particle sizes was tested in this experiment. The as-received MgO (referred to as mix in the report), and two MgO particle sizes with the highest weight fractions were used. The larger particle-size MgO had particles with diameters between 1.0 - 2.0 mm (mesh 10 and 18), which accounted for 32 wt % of the as-received MM MgO. The smaller particle-size MgO had particles with diameters less than 75 µm (mesh 200), which accounted for 18 wt % of the as-received MM MgO (see Section 3 of Deng et al., 2008).

Two WIPP-relevant MgO-to-brine ratios, 3 g/11 ml and 3.1 g/77 ml, were used in the long-term inundated-hydration experiments. Nemer (2006) has shown that a range of 0.001 g MgO/ml to 10 g MgO/ml brackets the expected range of MgO-to-brine ratios in WIPP. As shown in Nemer (2006), a more practical solid-to-liquid ratio is found by dividing the amount of MgO assumed to be emplaced in each panel by the minimum brine volume needed for a direct brine release (Stein, 2004). This solid-to-brine ratio is 4 g MgO/ml. However, we observed that 0.4 g MgO/ml of water was barely enough to cover the solids in the accelerated-inundated hydration experiment. Therefore we used a 3 g/11 ml ratio in the long-term hydration experiment. The 3.1 g MgO/ 77 ml brine MgO-to-brine ratio is comparable to the 5g MgO/100ml water MgO-to-water ratio used in our accelerated-inundated hydration experiments, which enables us to compare results.

Three brines were used in the experiment: GWB, ERDA-6 and simplified GWB. The brine GWB is a brine that approximates the brine in the Salado formation. The brine ERDA-6 is a brine that approximates the brine in the Castile formation. Simplified GWB is a brine that contains the major cations of GWB. SP 20-4 contains recipes and references for the three brines.

Table 1 describes the experimental matrix. The sample name reflects the brine, the MgO-to-brine ratio and MgO particle size used in the experiment. GW, ER, and MgCl represent the three brines: GWB, ERDA-6, and simplified GWB. Next the number 3 or 20 represents MgO-to-brine-ratio 3 g/11 ml or 3.1 g/77 ml. Last, the letters S, M, and L represent the MgO particle size: small (S), mixed (M, as received Martin Marietta MgO) or large (L). For example, GW3S means GWB brine, 3 g MgO/11 ml brine, small MgO particles. A serial number is also given to each sample to make the sample identification unique, such as GW3S1.

Table 1. Long-term inundated hydration experiment matrix

Experiment	ID	Brine	Particle Size[2]	MgO(g)/Brine (ml) Ratio (g/ml)[3]
1	GW3S	GWB	small	3/11
2	ER20S	ERDA-6	small	3.1/77
3	MgCl3S	Simplfied[1] GWB	small	3/11
4	GW20M	GWB	mix	3.1/77
5	ER3M	ERDA-6	mix	3/11
6	MgCl20M	Simplified GWB	mix	3.1/77
7	GW20L	GWB	large	3.1/77
8	ER3L	ERDA-6	large	3.1/77
9	MgCL20L	Simplified GWB	large	3.1/77
10	GW3M	GWB	mix	3/11
11	ER20M	ERDA-6	mix	3.1/77
12	MgCl3M	Simplified GWB	mix	3/11

1. Simplified GWB is a 1 M $MgCl_2$ + 3.6 M NaCl solution.
2. Particle size "large" represents MgO with diameters between 1.0 - 2.0 mm. Particle size "small" represents MgO with diameters less than 75μm. Particle size "mix" represents as received MgO, never sieved.
3. Samples with MgO/brine ratio 3/11 contained 3 ± 0.05g of MM MgO and 11 ± 1ml of brine. Samples with MgO/brine ratio 3.1/77 contained 3.1 ± 0.05g of MM MgO and 77 ± 2ml of brine.

2.2 Experimental Procedures

Martin Marietta MagChem 10 WTS MgO (MM MgO), which is currently being emplaced in WIPP, has been used throughout the experiment. Wheaton HDPE serum bottles (125 ml) or Nalgene HDPE centrifuge tubes (30 ml) containing brine and MM MgO were placed in a 28 °C incubator for the duration of the experiment. In order to accurately measure the MgO hydration rate, we performed loss-on-ignition (LOI) and carbon-coulometry tests on as-received MM MgO to determine if any MgO had been hydrated or carbonated before the hydration experiments were begun. The average brucite mole % in as-received MM MgO was found to be 0.19% ± 0.047%. The carbon wt % of MgO was tested by a UIC Inc CO_2 coulometer model CM504 with furnace apparatus model CM5120. The average carbon wt % was found to be 0.006% ± 0.002% which is at the detection limit of the instrument (see Section 3 of Deng et al., 2008).

The long-term inundated-hydration samples were collected at various times depending on the rate of hydration. After a sample is taken out of the incubator, the total weight (sample + container) and pH of each sample are quickly measured. The total weight of the sample is measured by a Mettler Toledo balance. The experiment started in February of 2007. Thus far, each sample has lost about 0.2-0.3 g over the 16 month period. A weight loss of 0.2-0.3 g is about 0.1% of the initial total weight for samples with MgO/brine ratio 3/11 or 0.01% for the samples with MgO/brine ratio 3.1/77. This indicates that our sample containers were well sealed against moisture loss. The solid portion of each sample was vacuum filtered using Whatman No. 40 filter paper, and rinsed with DI water to remove any remaining brine. The filtered solids were then dried at room temperature, at least over night. Samples were then ground and characterized by powder X-ray diffraction (XRD, see Subsection 3.1), and scanning electron microscopy (SEM) as described in Subsection 3.2.

A portion of the liquid from the sample bottles was analyzed by using an inductively coupled plasma atomic emission spectrometer (ICP-AES, Perkin Elmer DV 3300) to determine the concentration of dissolved Mg, and Ca. An Orion EA 940 pH/ion analyzer and Ross electrode were used to measure pH. The pH meter was calibrated by three pH buffers bracketing the sample pH range prior to measurement. Hydrogen-ion concentrations based on the pH reading and Gran titrations of the brines are reported in Subsection 4.4.

In order to gain more information on Mg-Cl-OH-hydrate formation, Cl^- concentration was monitored using an Orion EA 940 pH/ion analyzer using a Cl^- ion selective electrode (Orion model 96/7B). Chloride concentration was also measured using a Dionex 3000 ion chromatograph (IC) with AS23 4mm column and Ag23 4mm guard column. We found that Cl^- concentrations measured by a chloride electrode were not accurate for complex brines such as GWB or ERDA-6, thus only the IC measured Cl^- concentrations are used in the report.

3 EXPERIMENTAL RESULTS

3.1 Phase Identification Based on XRD Patterns

Phase identification of the crystalline phases present in the hydration product was performed using a D8 Advance Bruker X-ray diffractometer (XRD). All XRD patterns were collected using Cu Kα radiation at a scanning rate of 1.33°/min for a 2θ range of 10-90°. The detection limit for XRD is on the order of a few weight percent. XRD patterns for the long-term inundated hydration product are displayed in Figure 1 through Figure 12. Two detectors, Kevex and Sol-X have been used to collect the XRD patterns. Thus there are differences in the absolute peak intensities. Therefore the counts in the XRD patterns displayed in Figure 1 through Figure 12 should be considered qualitative. In this report XRD is only used to identify the mineral phases present in the samples and not to quantify the amount of each phase. In future work, the collected samples will be re-scanned using a single detector and the Rietveld method will be applied to quantify the wt% of mineral phases.

The hydration products include brucite and phase-5. MgO hydrated in simplified GWB or GWB produces phase-5 and brucite, while MgO hydrated in ERDA-6 produces brucite. Some halite (NaCl) is also observed in the XRD. Given that MgO hydration consumes water and all three brines have high concentrations of NaCl, it is reasonable to assume that halite precipitated out of solution.

Figure 1 through Figure 4 show that brucite was formed by MgO hydration in ERDA-6 brine. There is also a small un-identified peak around 2θ of 12°. Looking at Figure 1 – Figure 2, one can see that brucite formed at 113 days in the hydration reaction with large MgO particles with MgO-to-brine ratio equal to 3/11, while brucite formed in only 24 days for as-received MgO with the same MgO-to-brine ratio. Figure 3 shows that brucite formed at 24 days in the hydration samples with small MgO particles and MgO-to-brine ratio equal to 3.1/77, while Figure 4 shows that brucite formed at 113 days in as-received MgO with the same MgO-to-brine ratio.

Figure 5 - Figure 6 show that phase-5 and brucite were formed in MgO samples hydrated in GWB brine with MgO-to-brine ratio equal to 3/11. Phase-5 generally formed first, then brucite formed. Phase-5 appeared in hydration products at 24 days and brucite appeared in 113 days for as-received MgO (Figure 5). Phase-5 appeared in hydration products at 24 days and brucite appeared in 41 days for small-MgO particles in experiments (Figure 6). Phase-5 and brucite co-existed at 498 days (Figure 5 - Figure 6). However, as shown in Subsection 4.2, the saturation indices for this system are still high (i.e. >1). Thus we do not yet know whether these phases co-exist at equilibrium in this system. Phase-5 appeared in the hydration product of as-received MgO with MgO-to-brine ratio equal to 3.1/77 at 371 days (see Figure 8). Neither phase-5 nor brucite is evident in large-MgO-particle samples hydrated in GWB collected at 371 days (see Figure 7). It appears that in GWB brine, the MgO/ brine ratio has a strong effect on the hydration rate.

MgO hydrated faster in simplified GWB compared to the other two brines. Figure 9 - Figure 12 indicate that phase-5 formed at 24 days in all MgO samples hydrated in simplified GWB and that brucite was formed at 24 - 41 days. Figure 9 - Figure 12 also show phase-5 and brucite co-existing at 400+ days. In this case, as shown in Subsection 4.2, the saturation indices are lower than the GWB system. It will be interesting to look at the results at much longer times to see whether phase-5 and brucite do co-exist at equilibrium.

Figure 1 through Figure 12 show that the MgO particle size has an effect on the hydration kinetics. Small MgO particles form hydration products before large particles. The same trend was observed in the accelerated-MgO-hydration experiments carried out in de-ionized (DI) water at 70 °C (Deng et al., 2008).

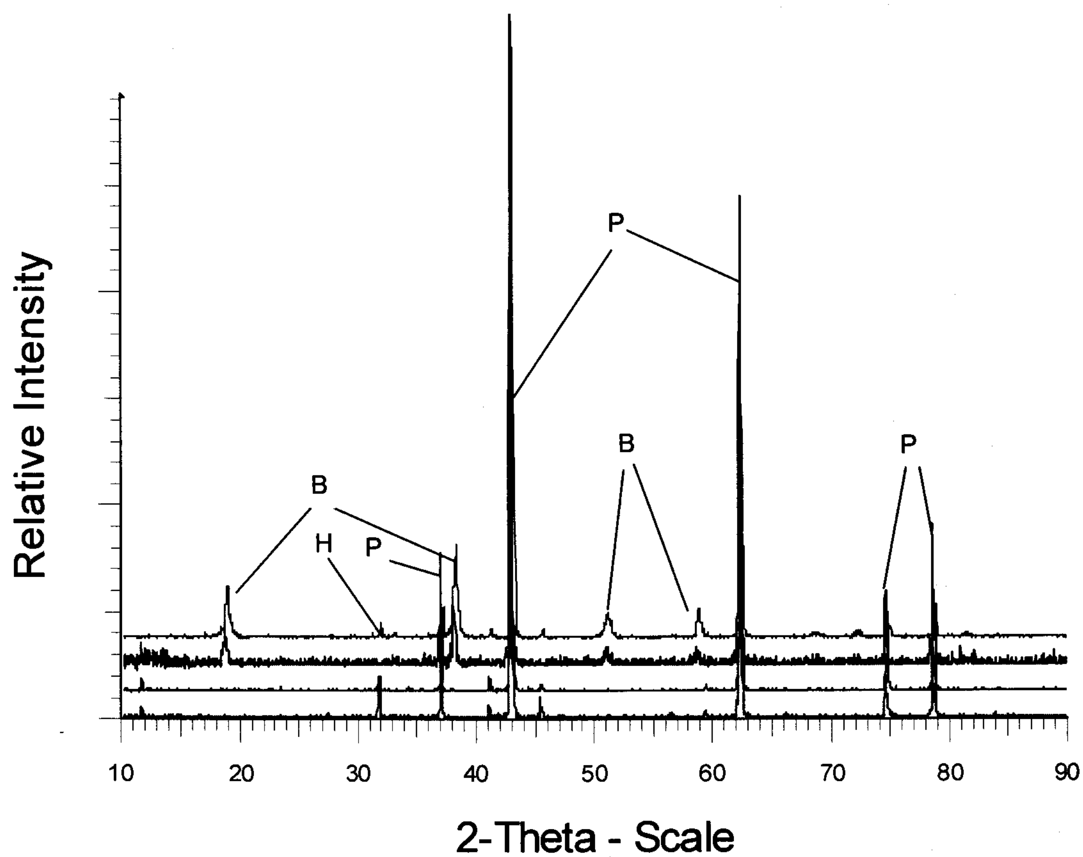


Figure 1. XRD of series ER3L, large MgO particles hydrated in ERDA-6 brine with MgO-to-brine ratio equal to 3 g/11 ml. Hydration products at 24, 50, 113, and 371 days are displayed in increasing vertical displacement upward in the figure. Here H indicates halite, B indicates brucite, and P indicates periclase. In the figure, brucite is first evident at 113 days.

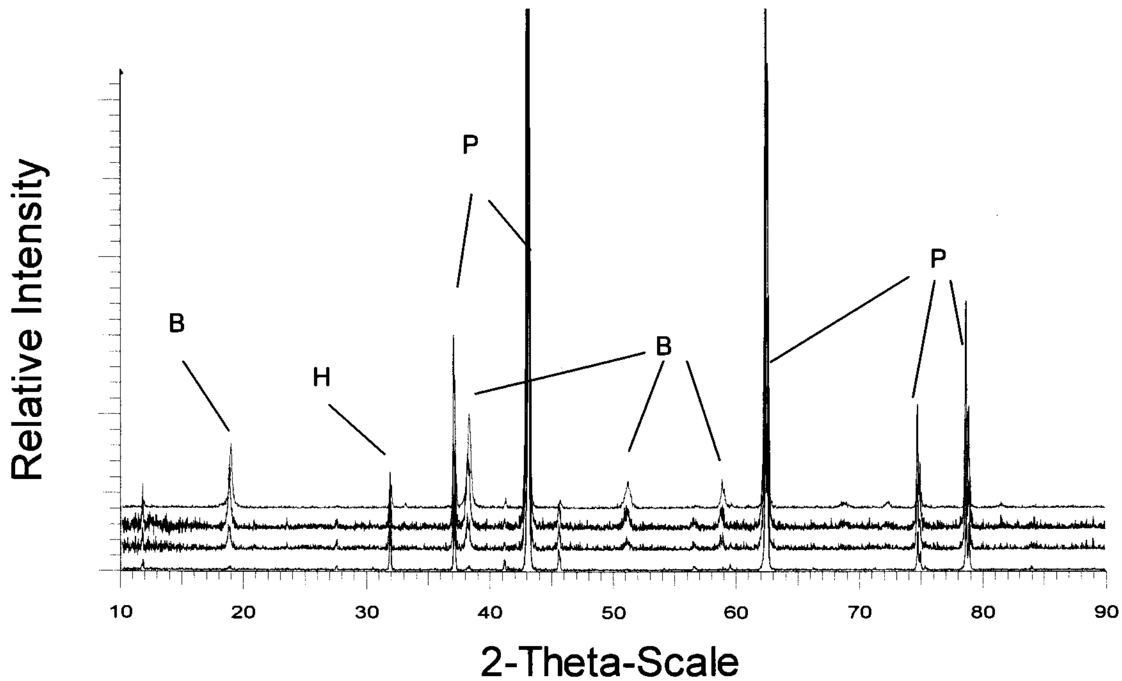


Figure 2. XRD of series ER3M, as-received MgO hydrated in ERDA-6 brine with MgO-to-brine ratio equal to 3 g/11 ml. Hydration products obtained at 24, 50, 113, and 371 days are displayed in increasing vertical displacement in the figure. Here H indicates halite, B indicates brucite, and P indicates periclase. In the figure, brucite is first evident at 50 days.

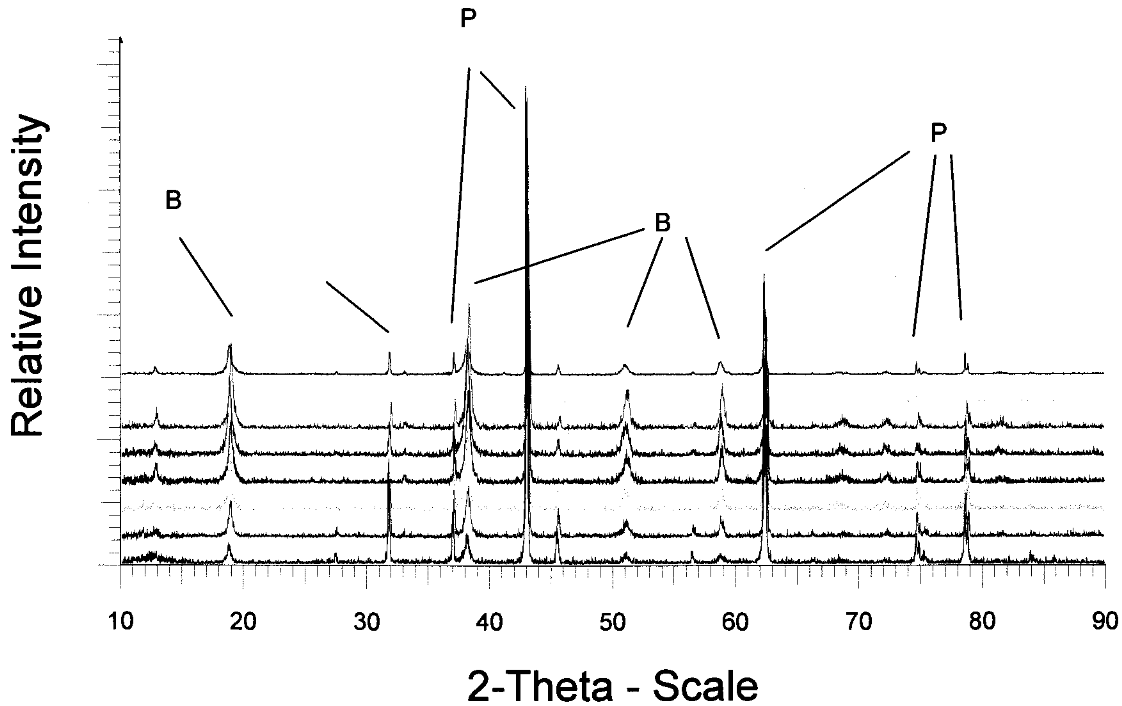


Figure 3. XRD of series ER20S, small MgO particles hydrated in ERDA-6 with MgO-to-brine ratio equal to 3.1 g/77 ml. Hydration products obtained at 24, 41, 50, 69, 113, 198, 308, and 498 days are displayed in increasing vertical displacement upward in the figure. Here H indicates halite, B indicates brucite, and P indicates periclase. In the figure, brucite is first evident at 24 days.

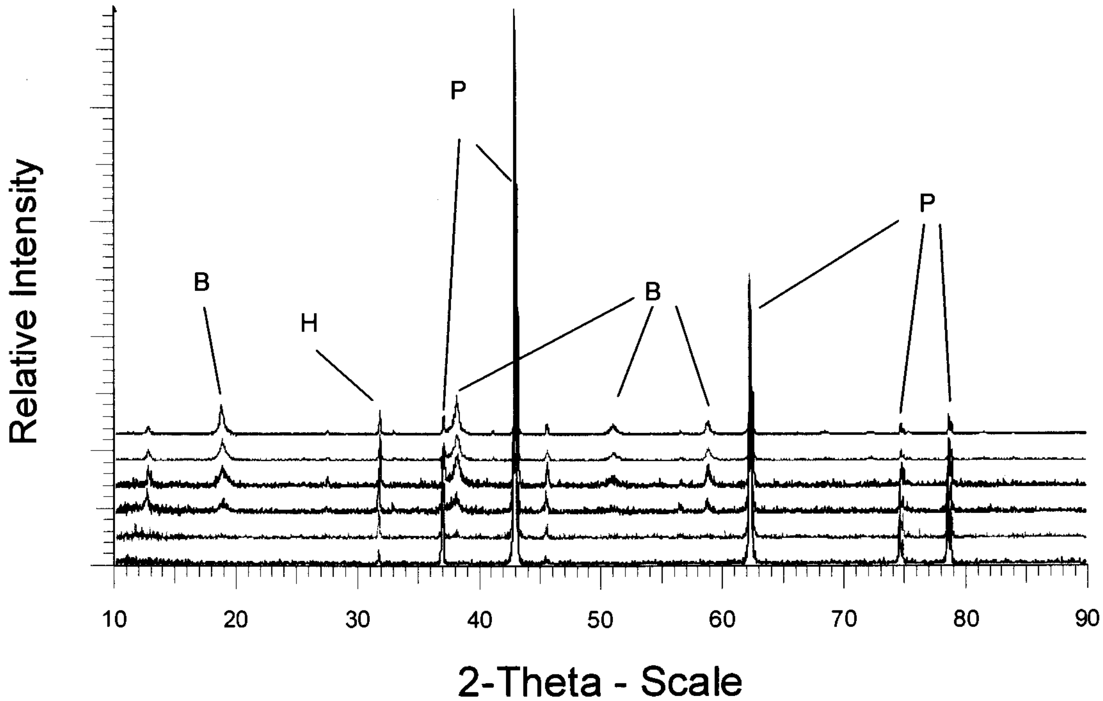


Figure 4. XRD of ER20M, as-received MgO hydrated in ERDA-6 brine with MgO-to-brine ratio equal to 3.1 g/77 ml. Hydration products obtained at 24, 50, 113, 198, 308, and 498 days are displayed in increasing vertical displacement upward in the figure. Here H indicates halite, B indicates brucite, and P indicates periclase. In the figure, brucite is first evident at 113 days.

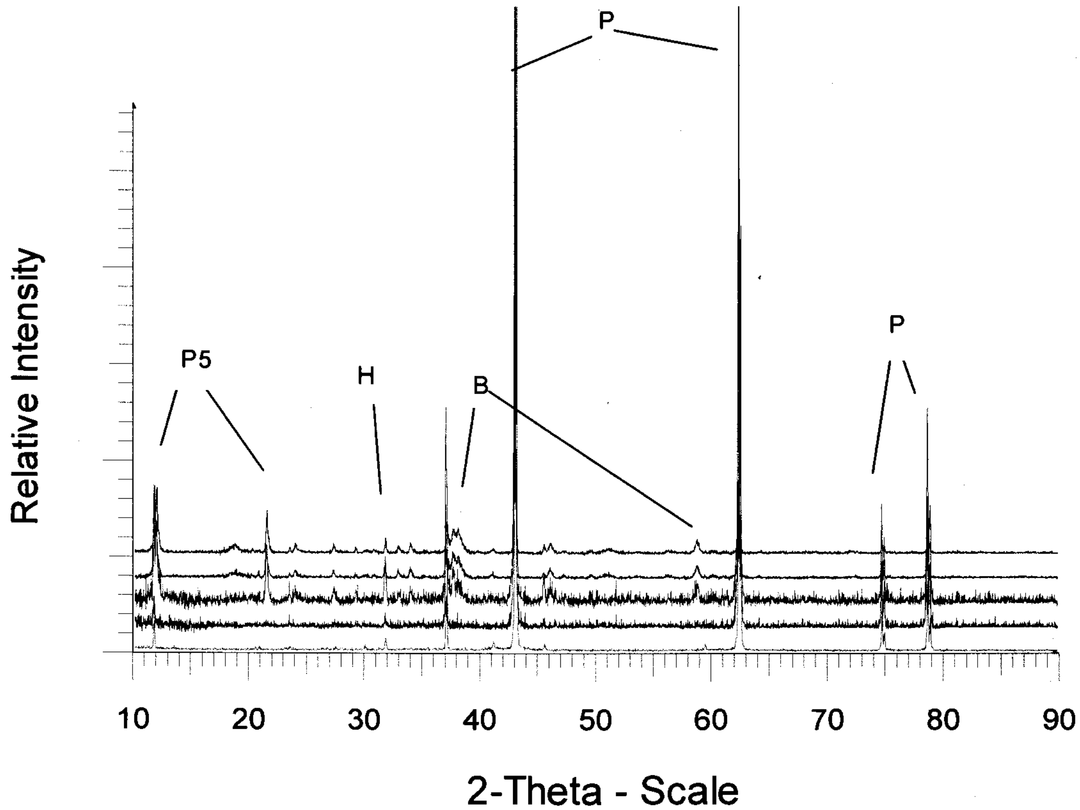


Figure 5. XRD of series GW3M, as received MgO hydrated in GWB brine with MgO-to-brine ratio equal to 3 g/11 ml. Hydration products obtained at 24, 50, 113, 198, and 498 days are displayed in increasing vertical displacement upward in the figure. Here P5 indicates phase-5, H indicates halite, B indicates brucite, and P indicates periclase. In the figure, phase-5 is first evident at 24 days and brucite is first evident at 113 days. At the latest collection date, 498 days, brucite and phase-5 are still co-existent.

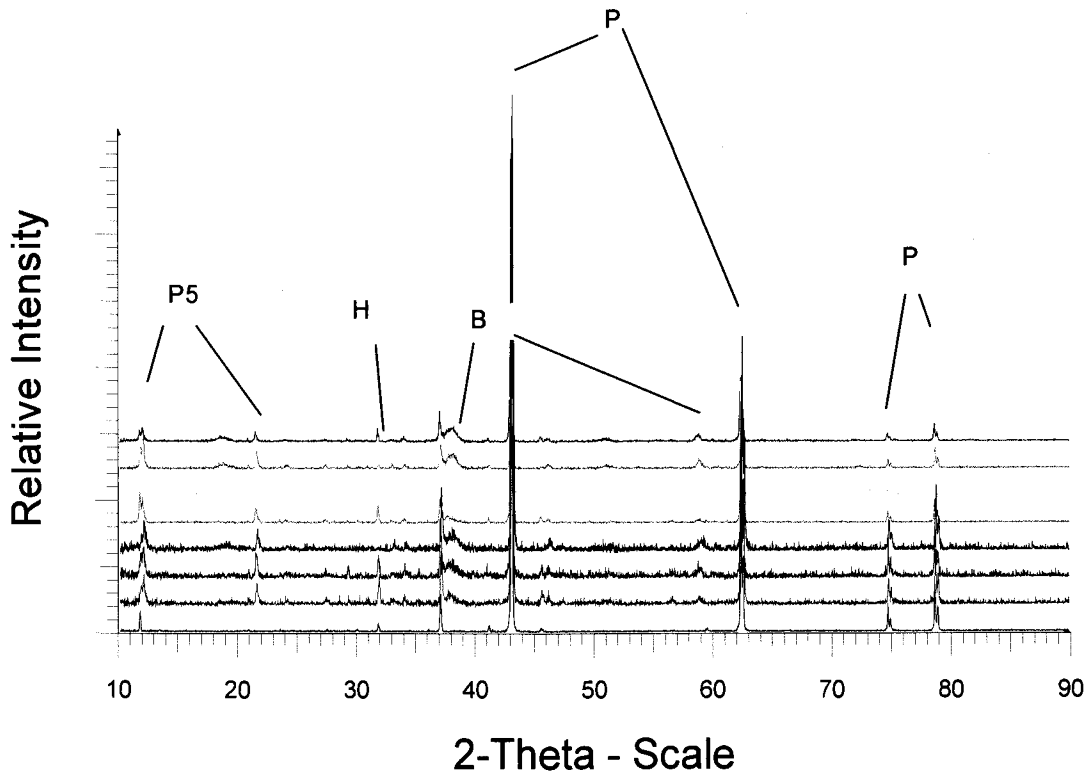


Figure 6. XRD of series GW3S, small MgO particles hydrated in GWB with MgO-to-brine ratio equal to 3 g/11 ml. Hydration products obtained at 24, 41, 50, 69, 113, 198, 308, and 498 days are displayed in increasing vertical displacement upward in the figure. Here P5 indicates phase-5, H indicates halite, B indicates brucite, and P indicates periclase. In the figure, phase-5 is first evident at 24 days, brucite is first evident at 41 days. At the latest collection date, 498 days, brucite and phase-5 are still co-existent.

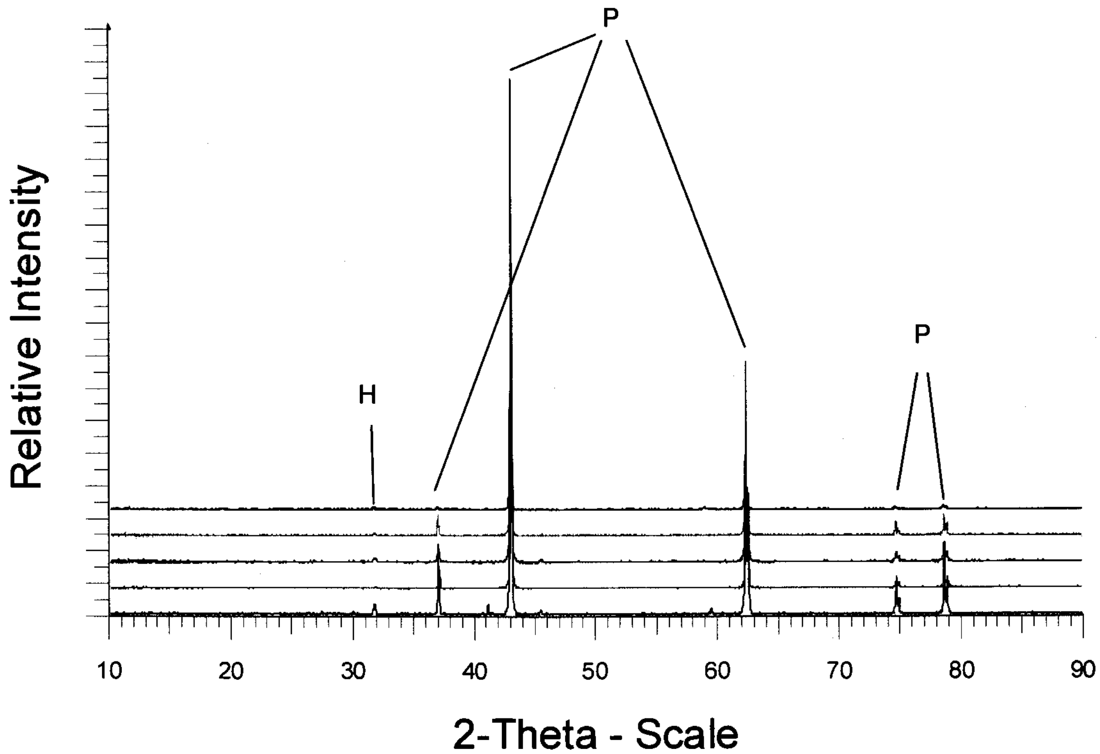


Figure 7. XRD of series GW20L, large MgO particles hydrated in GWB brine with MgO-to-brine ratio equal to 3.1 g/77 ml. Hydration products obtained at 24, 50, 113, 198, and 371 days are displayed in increasing vertical displacement upward in the figure respectively. Here H indicates halite, and P indicates periclase. Neither phase-5 nor brucite is observed.

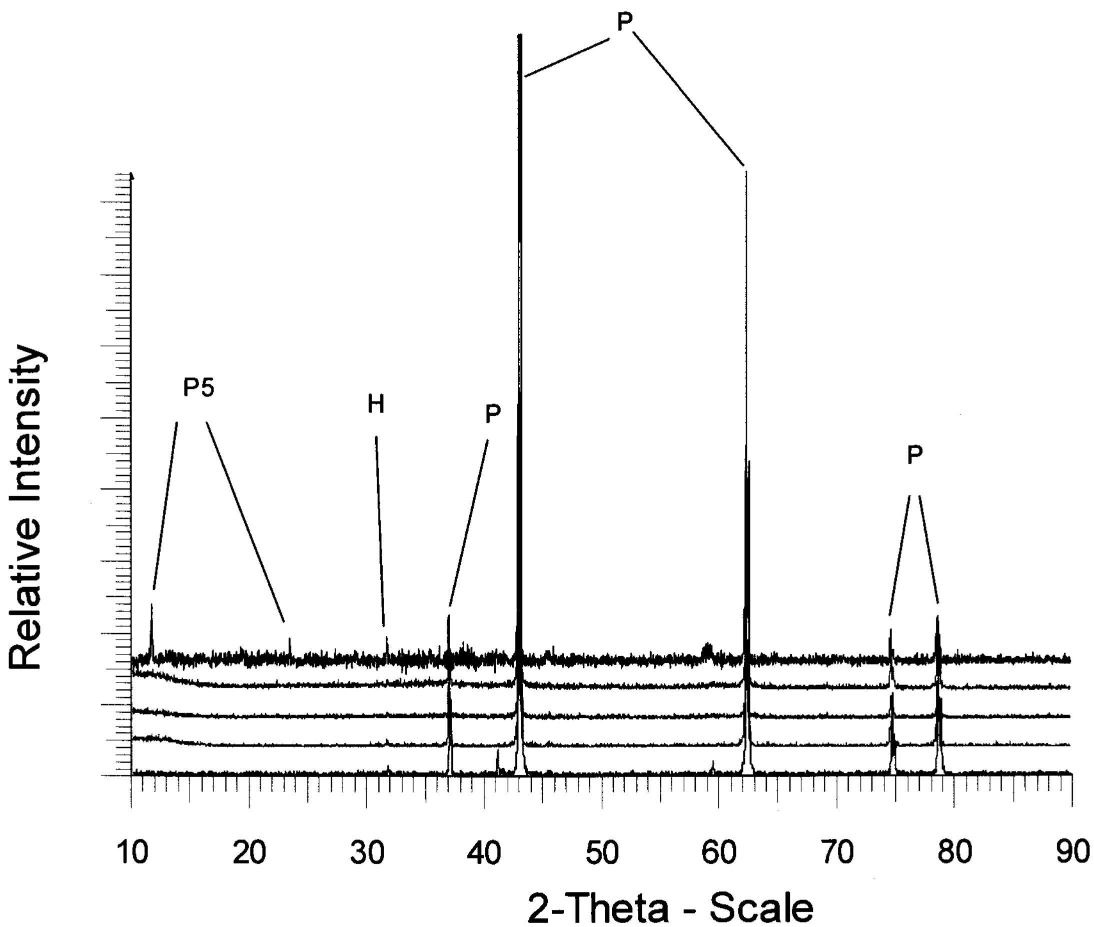


Figure 8. XRD of series GW20M, as received MgO hydrated in GWB brine with MgO-to-brine ratio equal to 3.1 g/77 ml. Hydration products obtained at 24, 50, 113, 198, and 371 days are displayed in increasing vertical displacement upward in the figure. Here P5 indicates phase-5, H indicates halite, B indicates brucite, and P indicates periclase. In the figure, phase-5 is evident at 371 days.

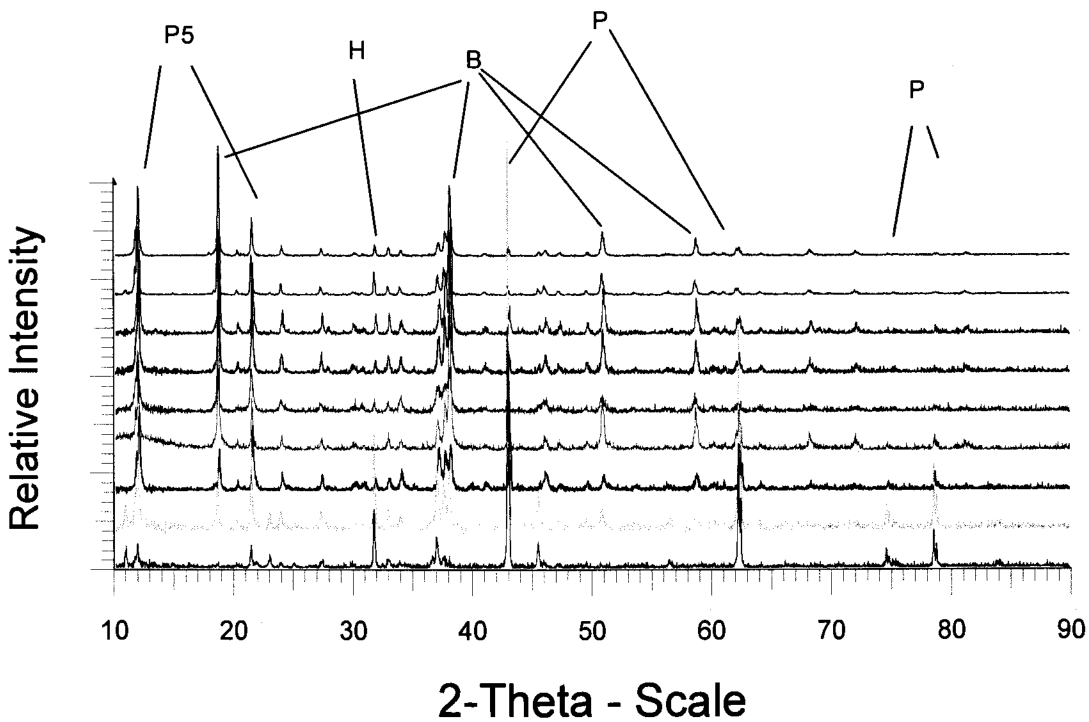


Figure 9. XRD of series MgCl20L, large MgO particles hydrated in simplified GWB brine with MgO-to-brine ratio equal to 3.1 g/77 ml. Hydration products obtained at 24, 41, 50, 113, 160, 198, 308, 436 and 498 days are displayed in increasing vertical displacement upward in the figure. Here P5 indicates phase-5, H indicates halite, B indicates brucite, and P indicates periclase. In the figure, phase-5 is first evident at 24 days and brucite is first evident at 41 days. At the latest collection, 498 days, brucite and phase-5 are still co-existent, and periclase is slightly visible.

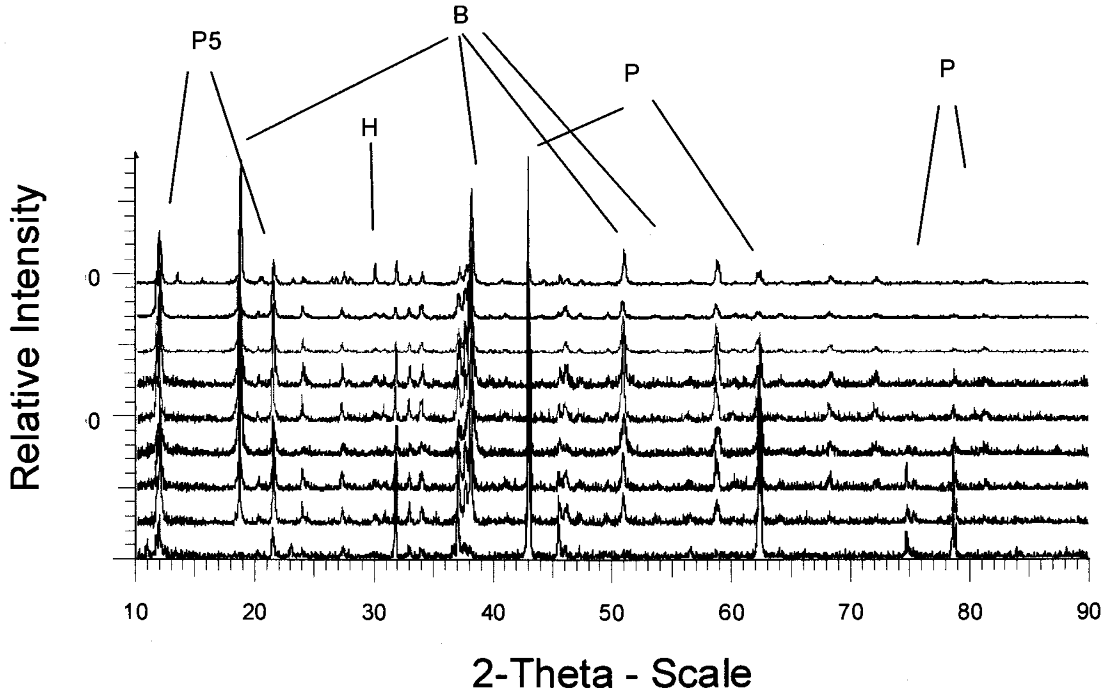


Figure 10. XRD of series MgCl3M3, as-received MgO hydrated in simplified GWB with MgO-to-brine ratio equals to 3 g/11 ml. Hydration products obtained at 24, 41, 50, 113, 160, 198, 308, 436, and 498 days are displayed in increasing vertical displacement upward in the figure. Here P5 indicates phase-5, H indicates halite, B indicates brucite, and P indicates periclase. In the figure, phase-5 is first evident at 24 days and brucite is first evident at 41 days. At the latest collection date, 498 days, brucite and phase-5 are still co-existent, and periclase is slightly visible.

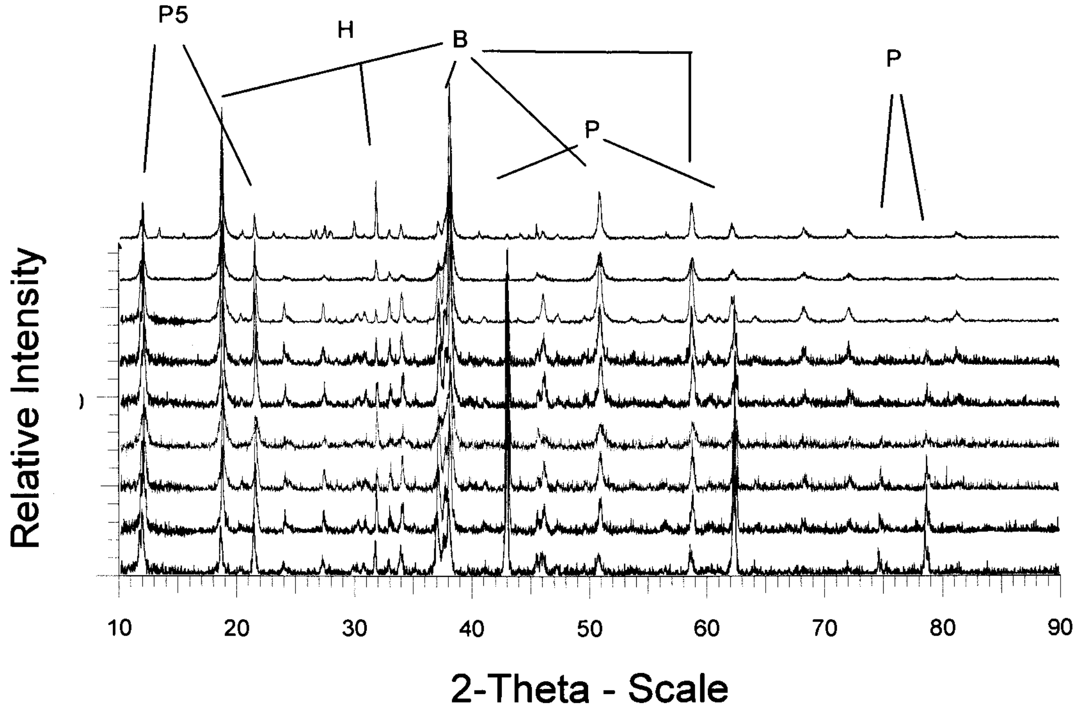


Figure 11. XRD of series MgCl3S, small MgO particles hydrated in simplified GWB with MgO-to-brine ratio equal to 3 g/11 ml. Hydration products obtained at 24, 41, 50, 113, 160, 198, 308, 436 and 498 days are displayed in increasing vertical displacement upward in the figure respectively. Here P5 indicates phase-5, H indicates halite, B indicates brucite, and P indicates periclase. In the figure, phase-5 and brucite are first evident at 24 days. At the latest collection date, 498 days brucite and phase-5 are still co-existent, and periclase is slightly visible.

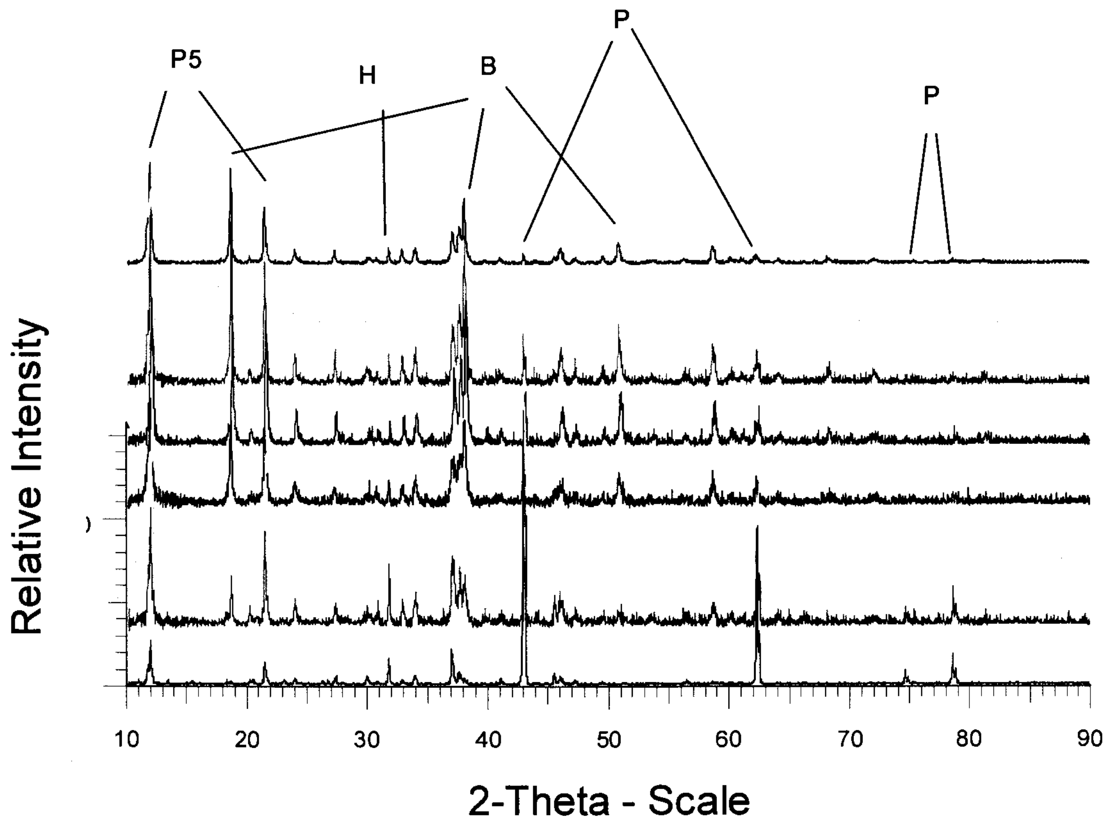


Figure 12. XRD of series MgCl20M, as received MgO hydrated in simplified GWB with MgO-to-brine ratio equal to 3.1 g/77 ml. Hydration products obtained at 24, 41, 50, 113, 160, 198, 308, and 436 days are displayed in increasing vertical displacement upward in the figure respectively. Here P5 indicates phase-5, H indicates halite, B indicates brucite, and P indicates periclase. In the figure, phase-5 is first evident at 24 days and brucite is first evident at 41 days. At the latest collection date, 436 days, brucite and phase-5 are still co-existent, and periclase is slightly visible.

3.2 SEM

To gain some understanding of the phases that are present in the MgO hydration product, SEM images were obtained using a JEOL JSM-5900LV with Energy Dispersive Spectroscopy (EDS). Samples were mounted on graphite tape and imaged.

Figure 13 and Figure 13A show SEM images of as-received MM MgO. The material is composed of large (10 μm) particles with smaller particles filling in the interstitial spaces.

Figure 14 - Figure 15 show SEM images of as received MgO particles that had been hydrated in ERDA-6 brine for 113 days. Figure 15 shows that a hydration product has been formed on the exterior of the particles. The XRD of as-received MgO hydrated in ERDA-6 (Figure 2) indicates that the hydration product is likely brucite.

Figure 16 - Figure 17 show SEM images of small MgO particles (i.e. particles initially < 75 μm) that have been hydrated in ERDA-6 for 308 days. The XRD of small MgO particles hydrated in ERDA-6 (Figure 3) indicates the sail-like crystals are most likely brucite.

Figure 18 shows an SEM image of a MgO particle that has been hydrated in GWB brine for 50 days. Regions (1) and (2a) show a fine carpet of needle like fibers that cover the external surface of the particle. A detailed view of these fibers is given in Figure 19. Evidence suggests that these needles are phase-5 ($Mg_3(OH)_5Cl{\cdot}4H_2O$), based on their morphology (which matches that of the literature, see Tooper and Cartz 1966), EDS spectra (Figure 20), and the powder XRD on this sample (Figure 6).

Figure 21 shows another region in the interior of the particle shown in Figure 18. A large un-reacted periclase particle is nested in a mass of smaller periclase particles and hydration products. Needles are also visible in the interior of the particle which is blown up in Figure 22. Figure 23 shows a detailed view of the granular fabric inside the particle. The figure shows that hydration has occurred throughout the particle, as the interstitial spaces have been filled with hydration products.

Figure 24 -Figure 25 show as-received MM MgO hydrated in simplified GWB for 113 days. Needles that are similar to that seen in GWB are visable but the needles in simplified GWB appear more coarse.

Figure 26 - Figure 27 show images of GW20L (GWB brine, 3.1 g/77 ml solid-to-liquid ratio, large particles) after hydration for 371 days. Upon looking at SEM images, one can see a thin (10 μm) coating of hydration product on the exterior of the particles. Figure 27 shows a network of fractures in the hydration product through which water can permeate. Thus we tentatively conclude that hydration is occurring in this set of experiments, albeit at a slower rate. The detection limit of XRD is on the order of a few weight percent, which may explain why no hydration product is observed in the XRD of the GW20L series (Figure 7).

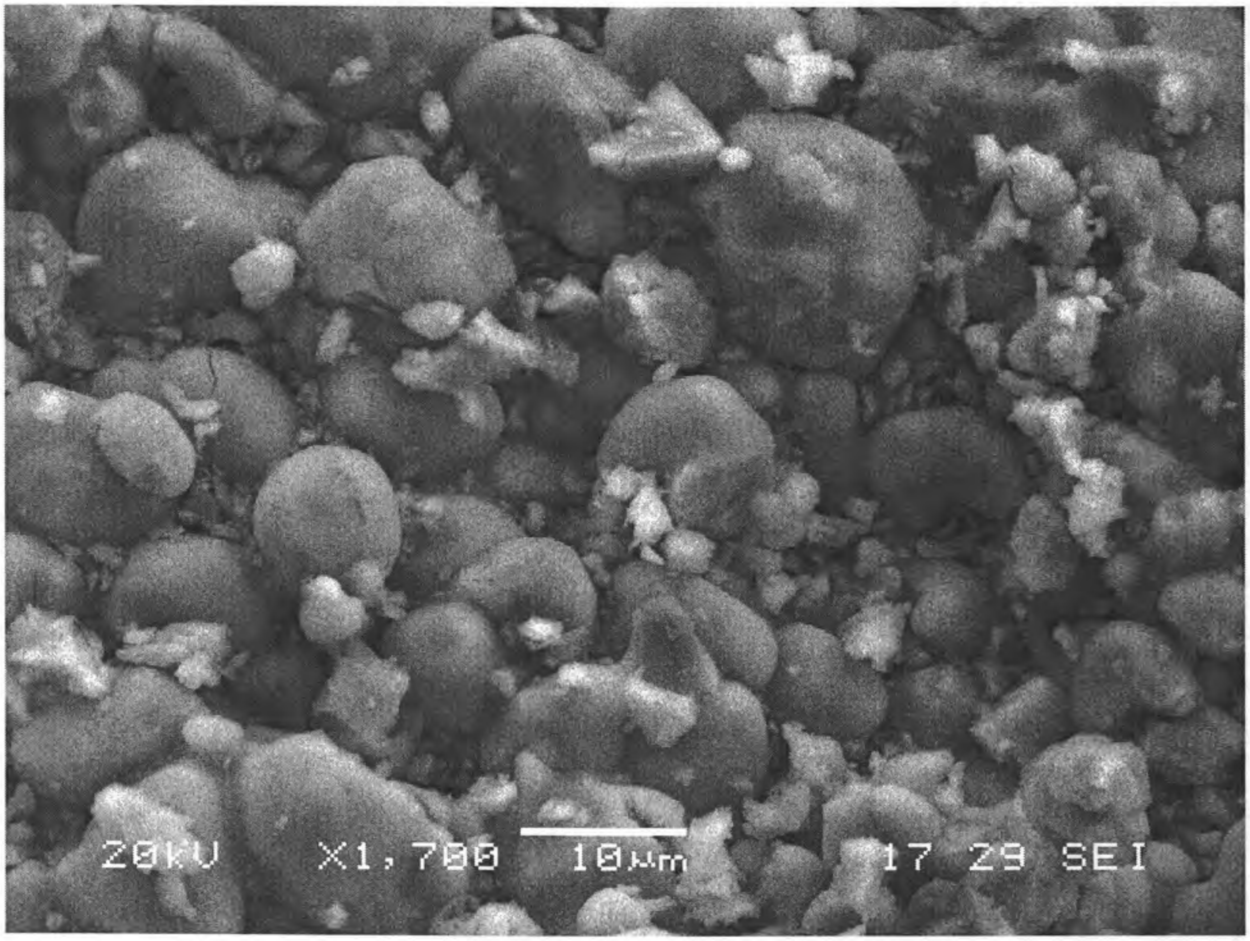


Figure 13. SEM image of as-received-MgO particles before hydration. This image is recorded as 816H4I4A.TIF in SN WIPP-MM MgO-2.

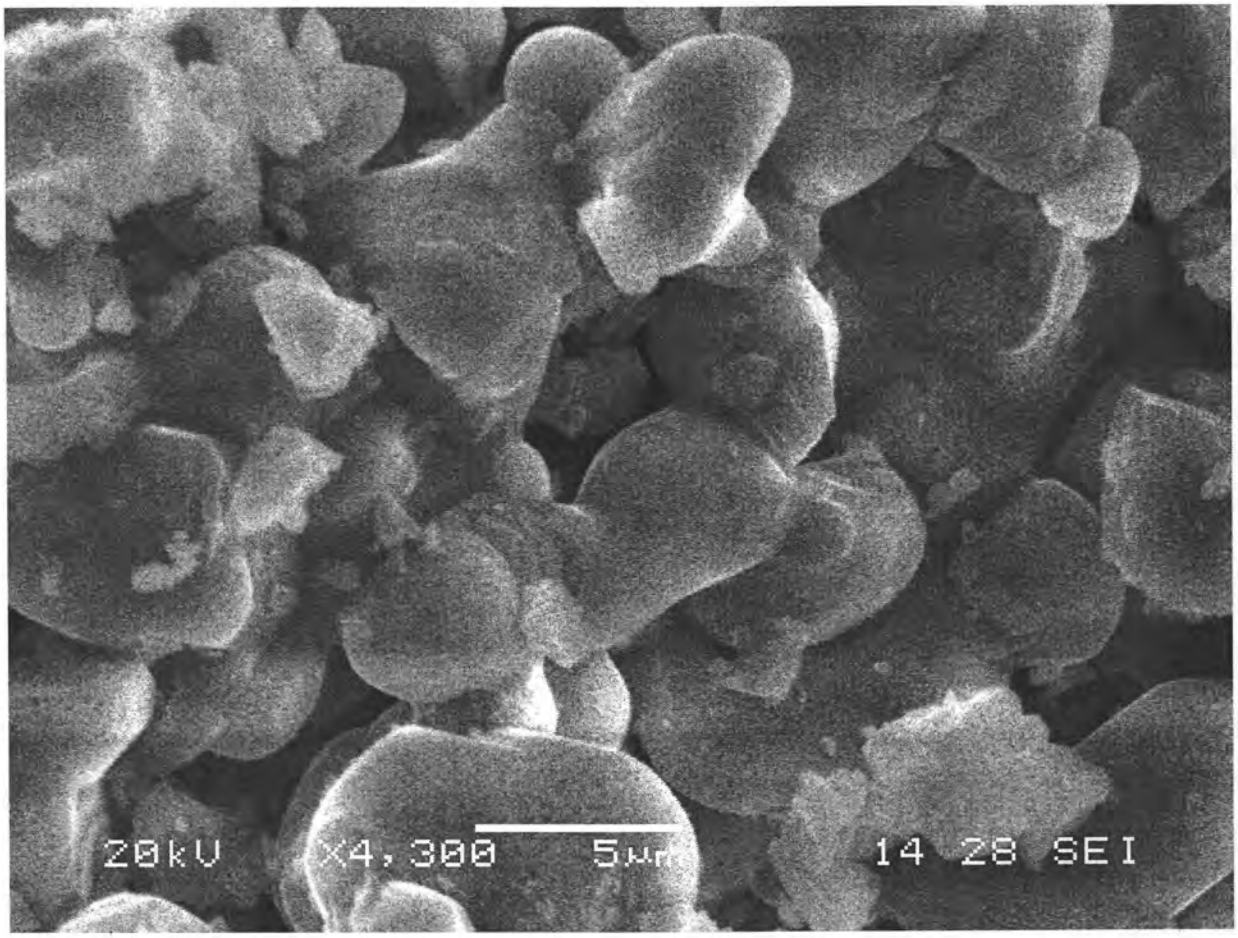


Figure 13A. SEM image of as-received-MgO particles before hydration (not same sample as Figure 13). Notice the change that occurs in the interstitial spaces during hydration between this image and Figure 23. This image is recorded as I1.BMP in SN WIPP-MM MgO-15, pg. 30.

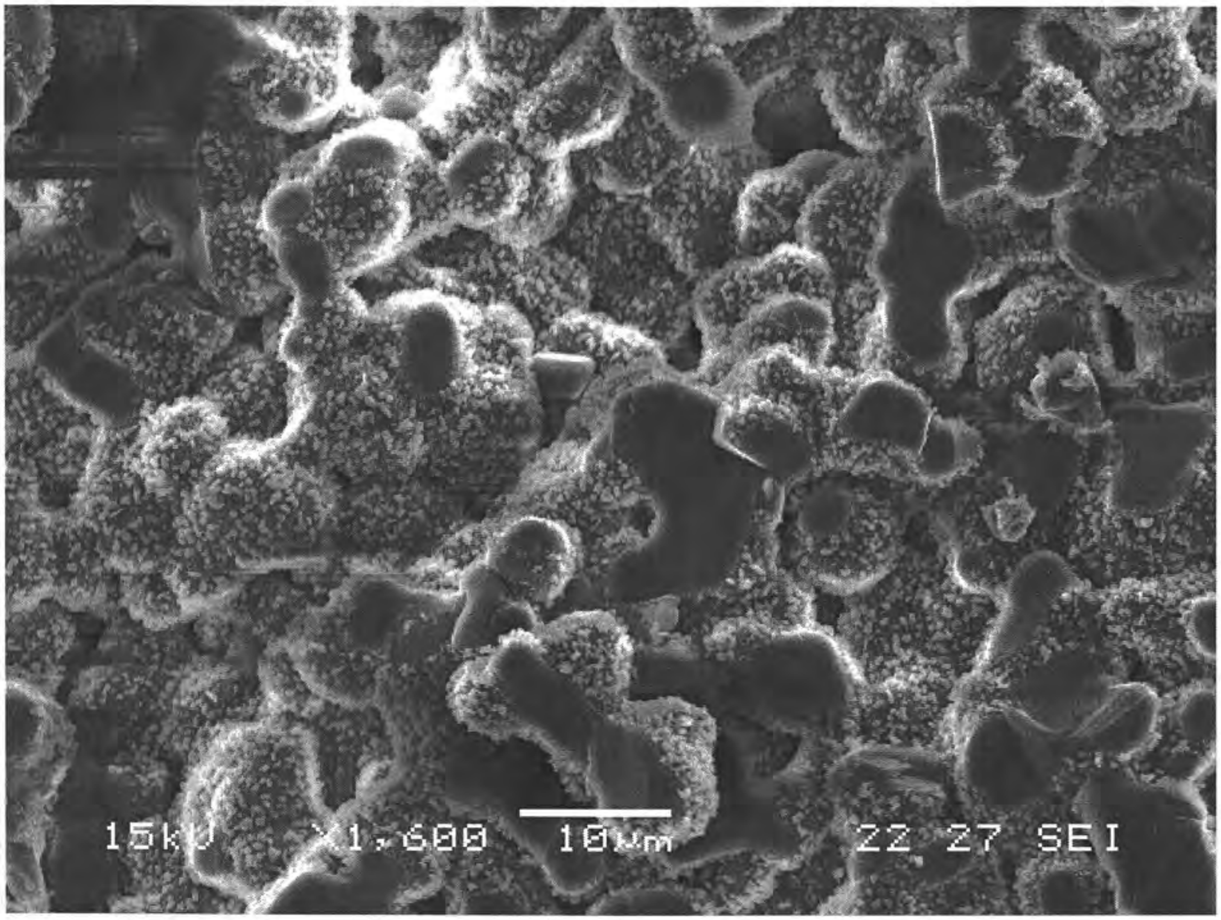


Figure 14. SEM image of a sample of series ER3M, as-received MgO hydrated in ERDA-6 brine with MgO-to-brine ratio equal to 3 g/11 ml for 113 days. This image is recorded as image H2I2C.bmp in SN WIPP-MM Mg0-8, pg. 17.

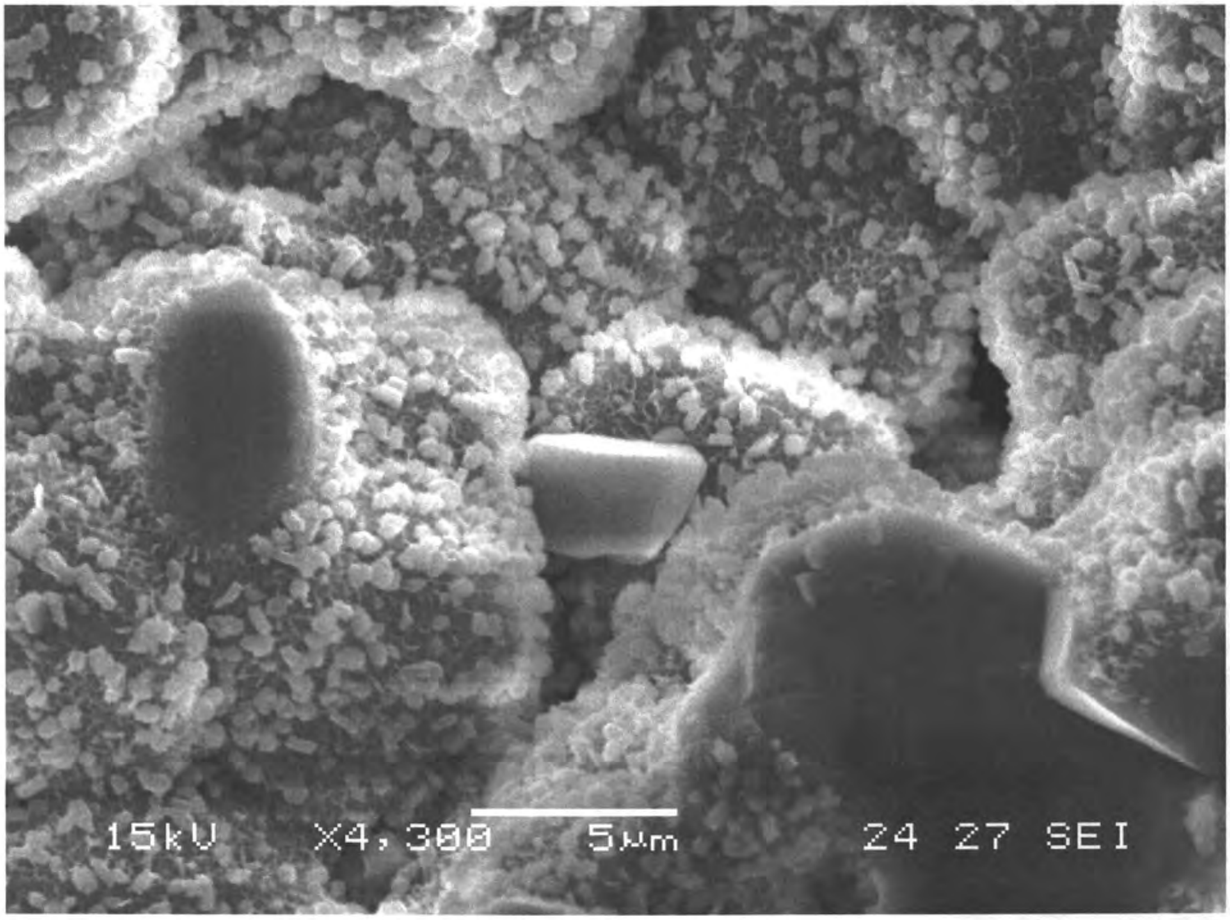


Figure 15. Higher magnification of Figure 14. The large particles are periclase with hydration product that is likely brucite growing on the exterior. The clean particle in the center of the image is halite. This image is recorded as H2I2B.bmp in notebook WIPP-MM MgO-8, pg. 17.

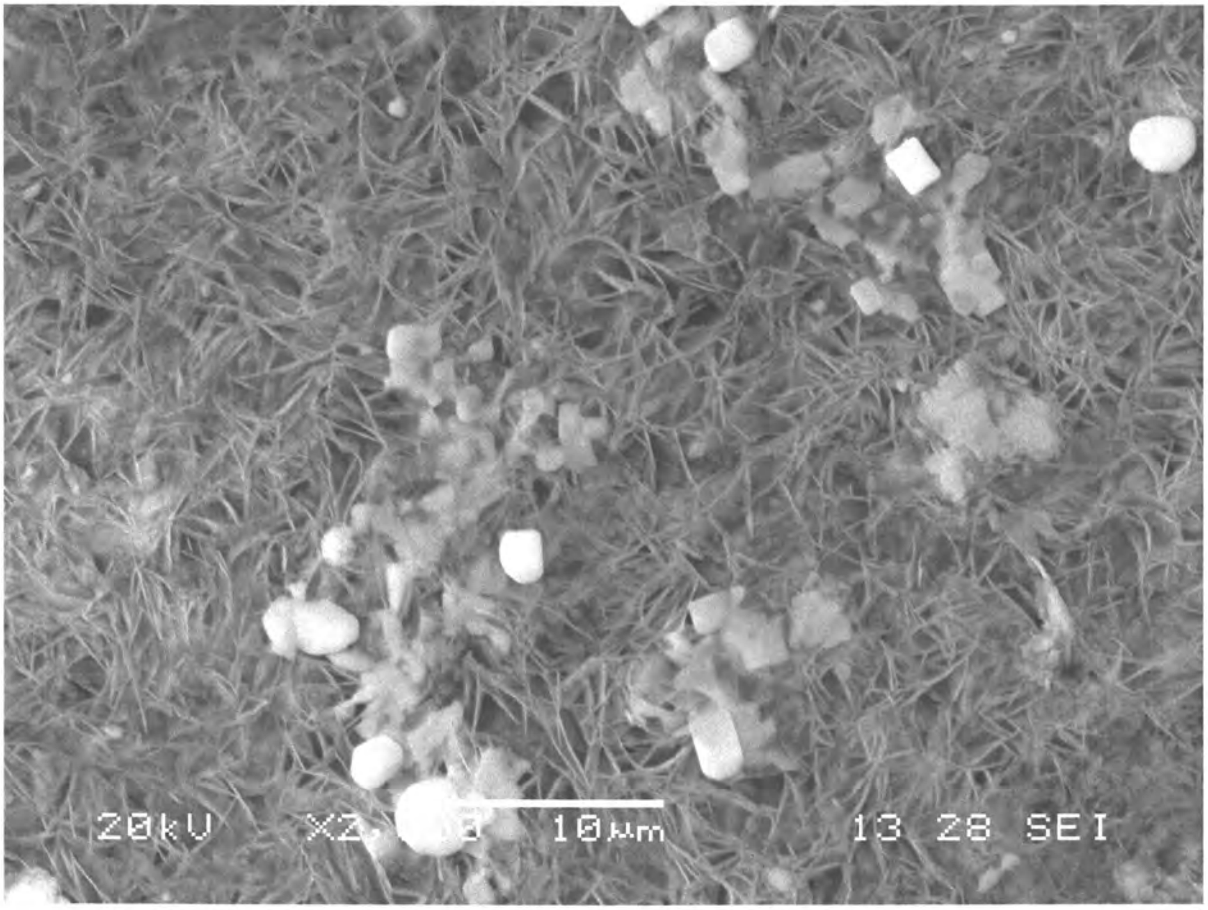


Figure 16. SEM image of a sample of series ER20S, small-MgO particles hydrated in ERDA-6 with MgO-to-brine ratio equal to 3.1 g/77 ml for 308 days. This image is recorded as I4.bmp in notebook WIPP-MM MgO-15, pg. 31.

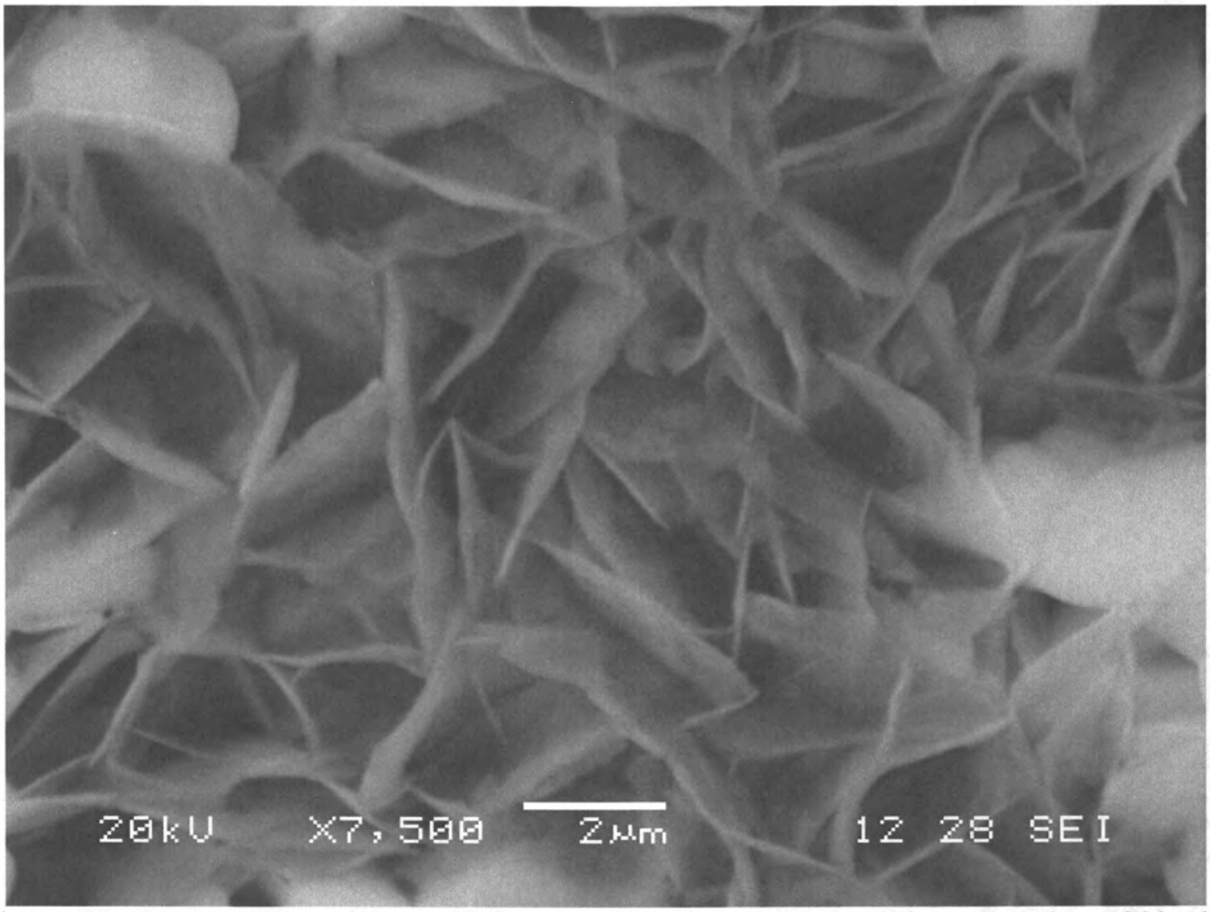


Figure 17. Same as Figure 16, at a different scale and at a slightly different location within the same particle. This image is recorded as I1A.bmp in notebook WIPP-MM MgO-15, pg. 31.

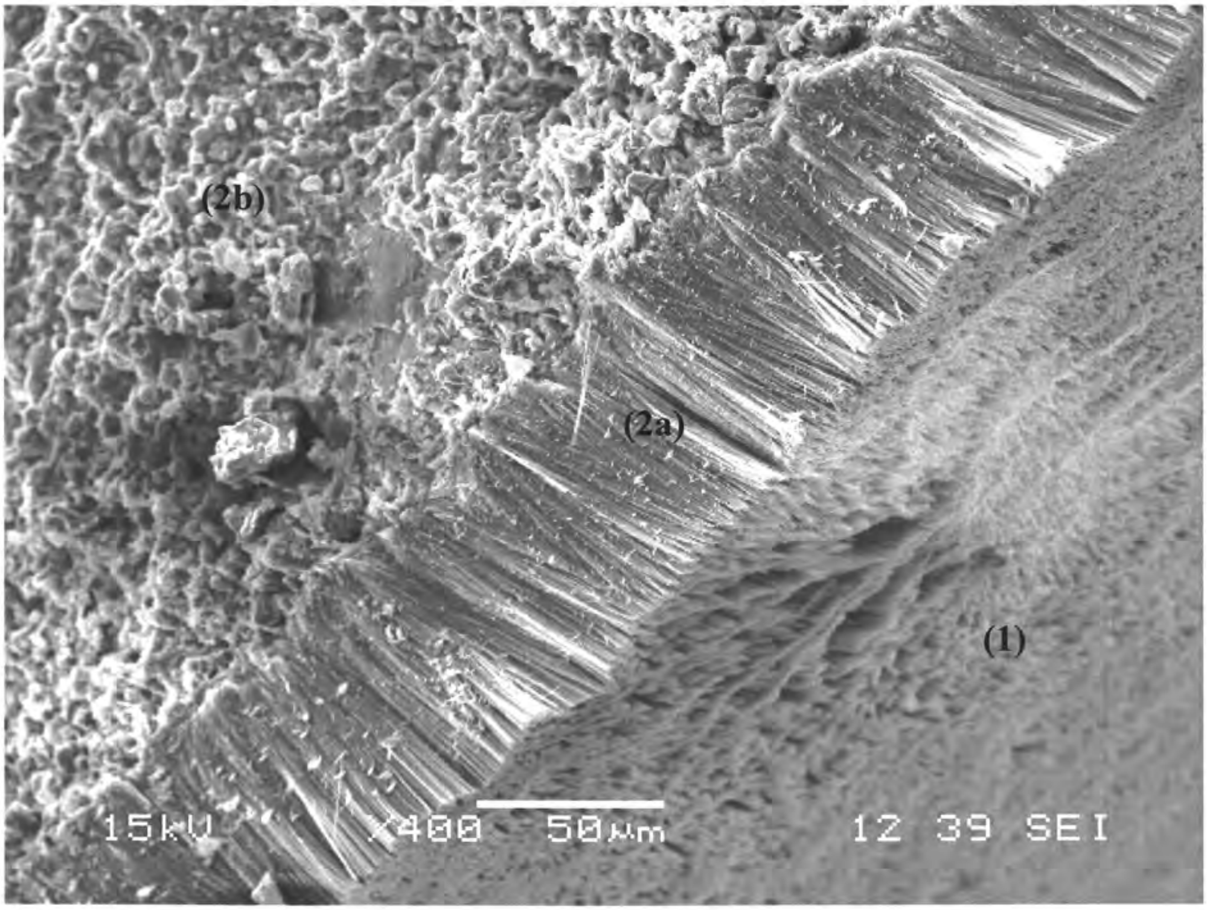


Figure 18. SEM image of a sample of series GW3S, small MgO particles hydrated in GWB brine with MgO-to-brine ratio equal to 3 g/11 ml for 50 days. Here the particle has been sliced open where region (1) is the external surface of the particle and (2a), (2b) are in the plane of the slice. This image is recorded as H1I4.BMP in SN WIPP-MM MgO-7, pg. 16.

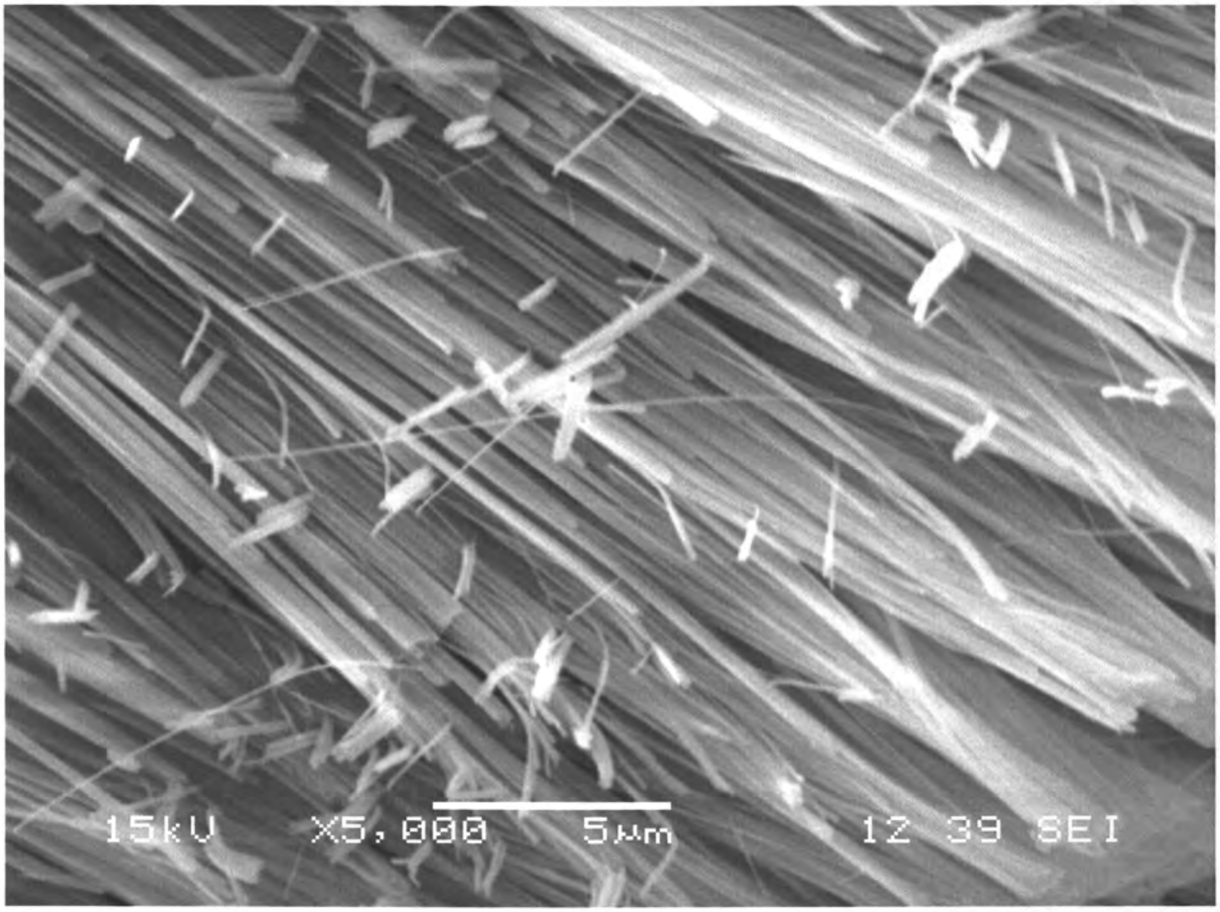


Figure 19. SEM image showing the detailed view of region (2a) from Figure 18. As explained in the text, the EDS spectra shown in Figure 20 indicates that the needle like fibers are likely phase-5. This image is recorded as H1I4B.BMP in SN WIPP-MM MgO-7, pg. 16.

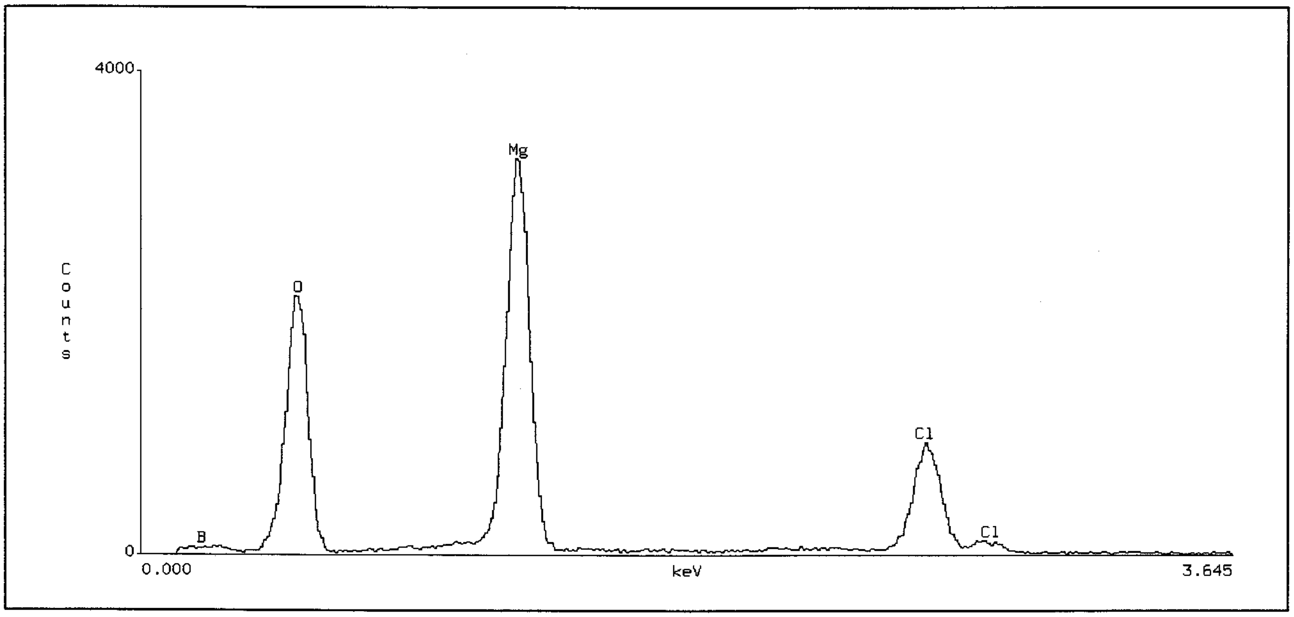


Figure 20. EDS spectra of area shown in Figure 19. This spectrum is recorded as H1I4S1B.EDS in SN WIPP-MM MgO-7, pg. 16.

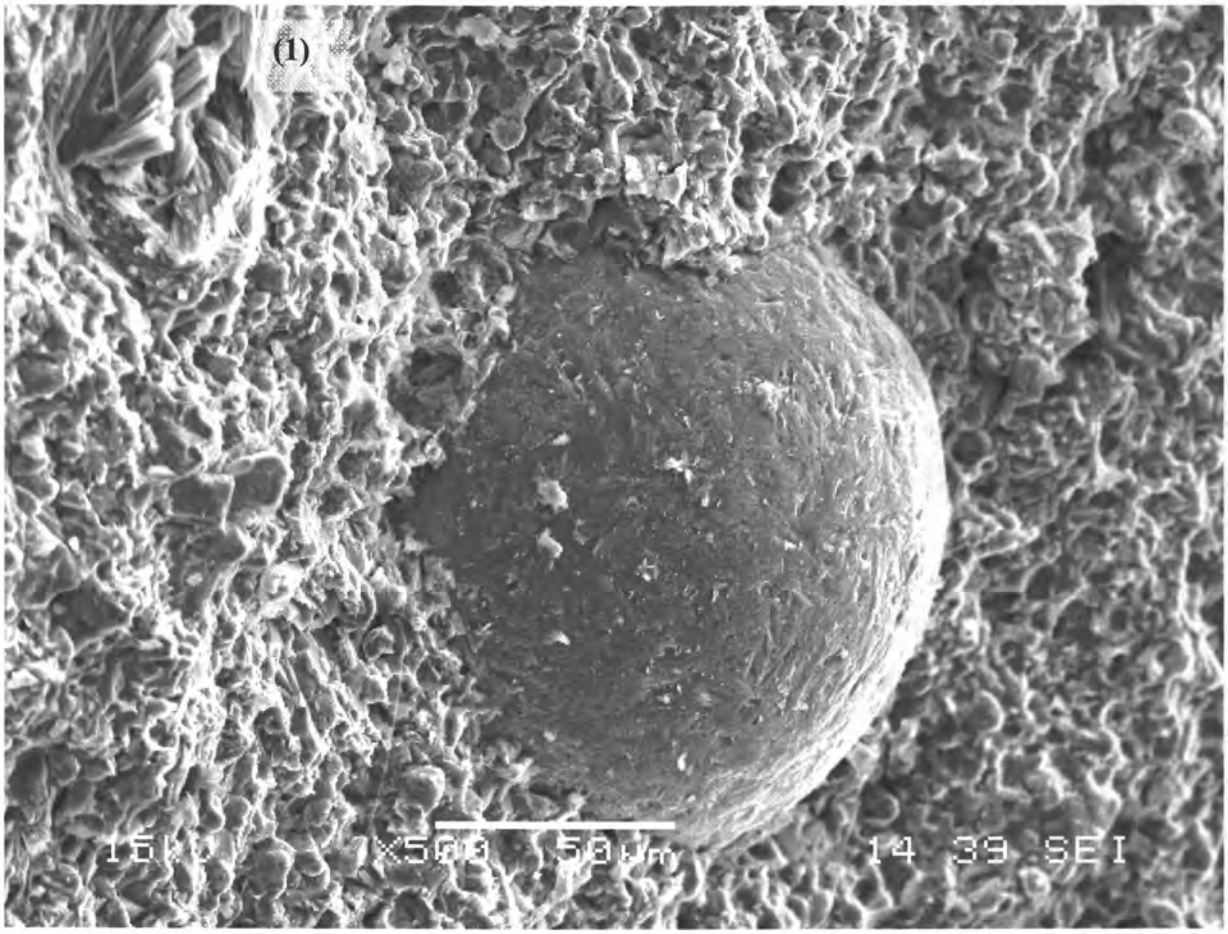


Figure 21. Interior of MgO particle shown in Figure 18. In the center of this image is a piece of partially reacted periclase surrounded by smaller pieces of partially reacted periclase and hydration products. A detailed view of region (1) is shown in Figure 22. A detailed view of the interior fabric is shown in Figure 23. This image is recorded as H1I1.BMP in SN WIPP-MM MgO-7, pg. 16.

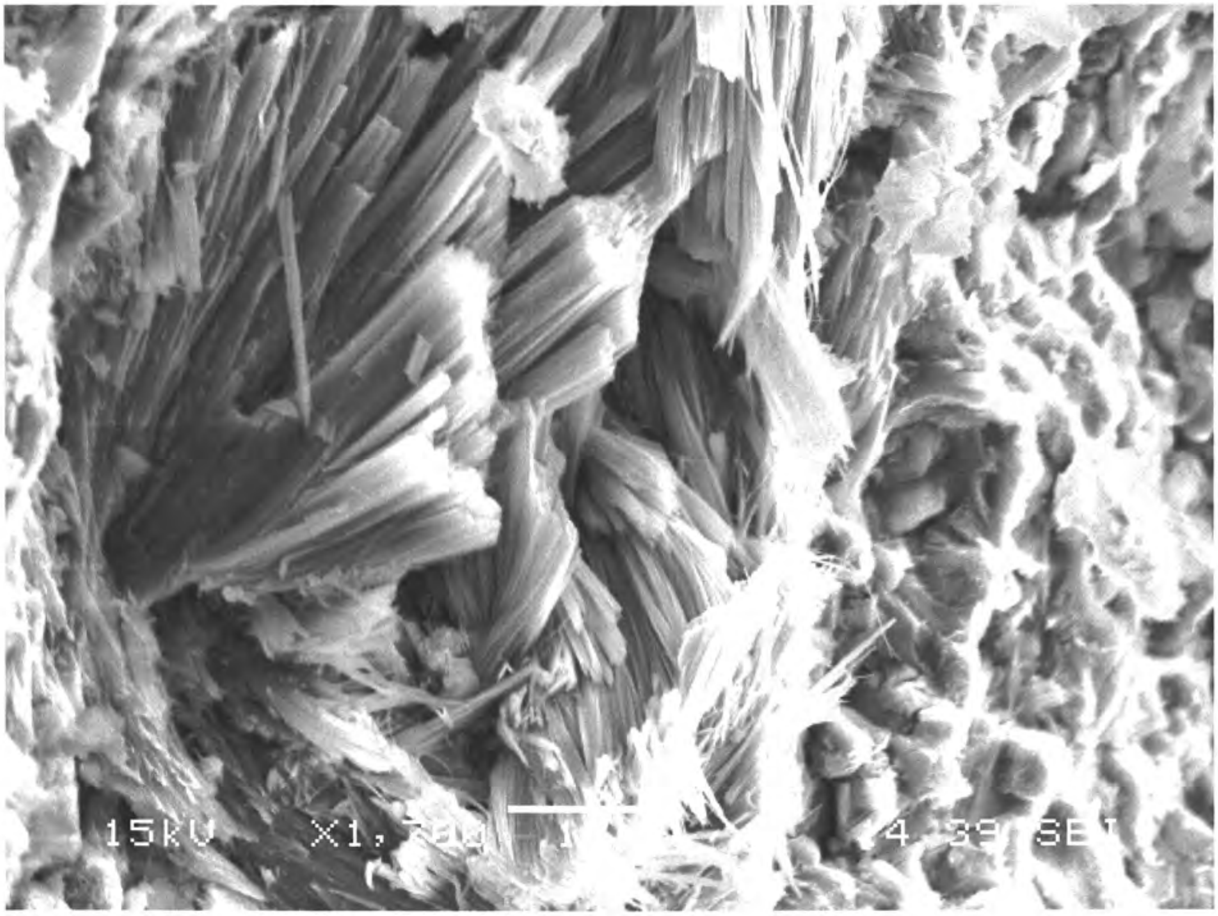


Figure 22. Detailed view of region (1) in Figure 21. These needles strongly resemble the outer carpet shown in Figure 18 and Figure 19. This image is recorded as H1I2.BMP in SN WIPP-MM MgO-7, pg. 16.

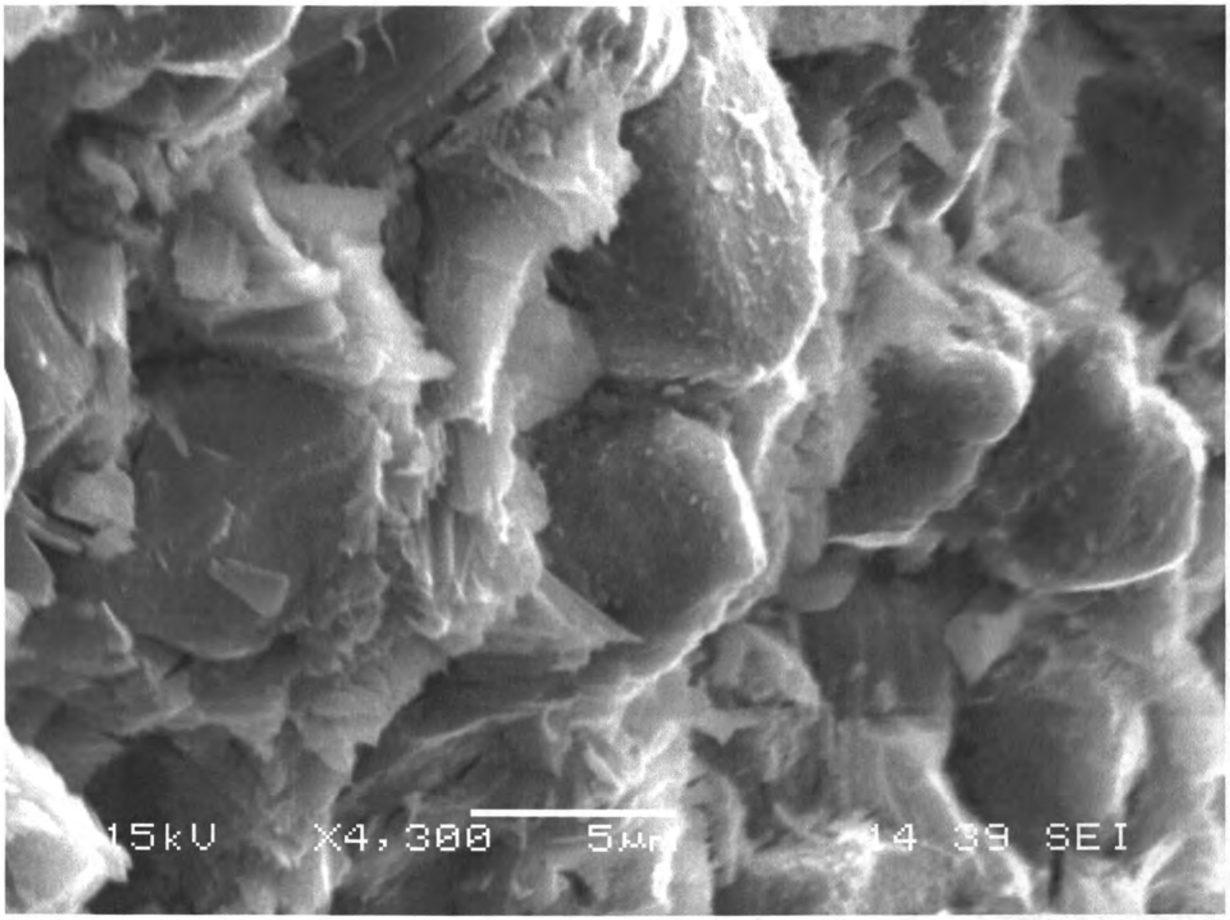


Figure 23. Detailed view of the interior of a partially hydrated MgO particle. The more rounded particles are periclase and the interstitial spaces have been filled with hydration products. See Figure 13 to examine as-received MgO particles before hydration. This image is recorded as H1I3.BMP in SN WIPP-MM MgO-7, pg. 16.

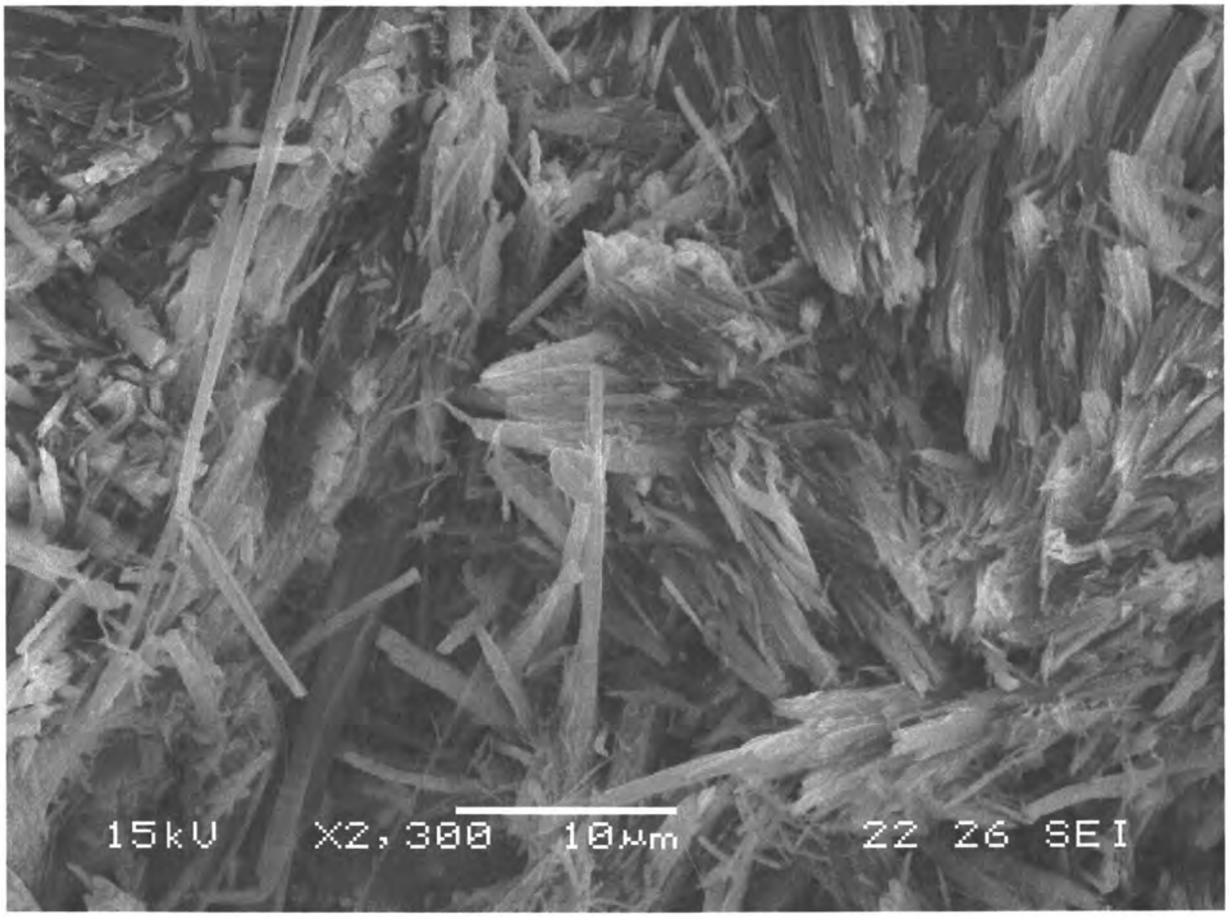


Figure 24. SEM image of a sample of series MgCl3M, as-received MgO particle after hydration in simplified GWB brine with MgO-to-brine ratio equal to 3 g/11 ml for 113 days. This image is recorded as H1I1.BMP in SN in WIPP-MM MgO-7, pg. 57.

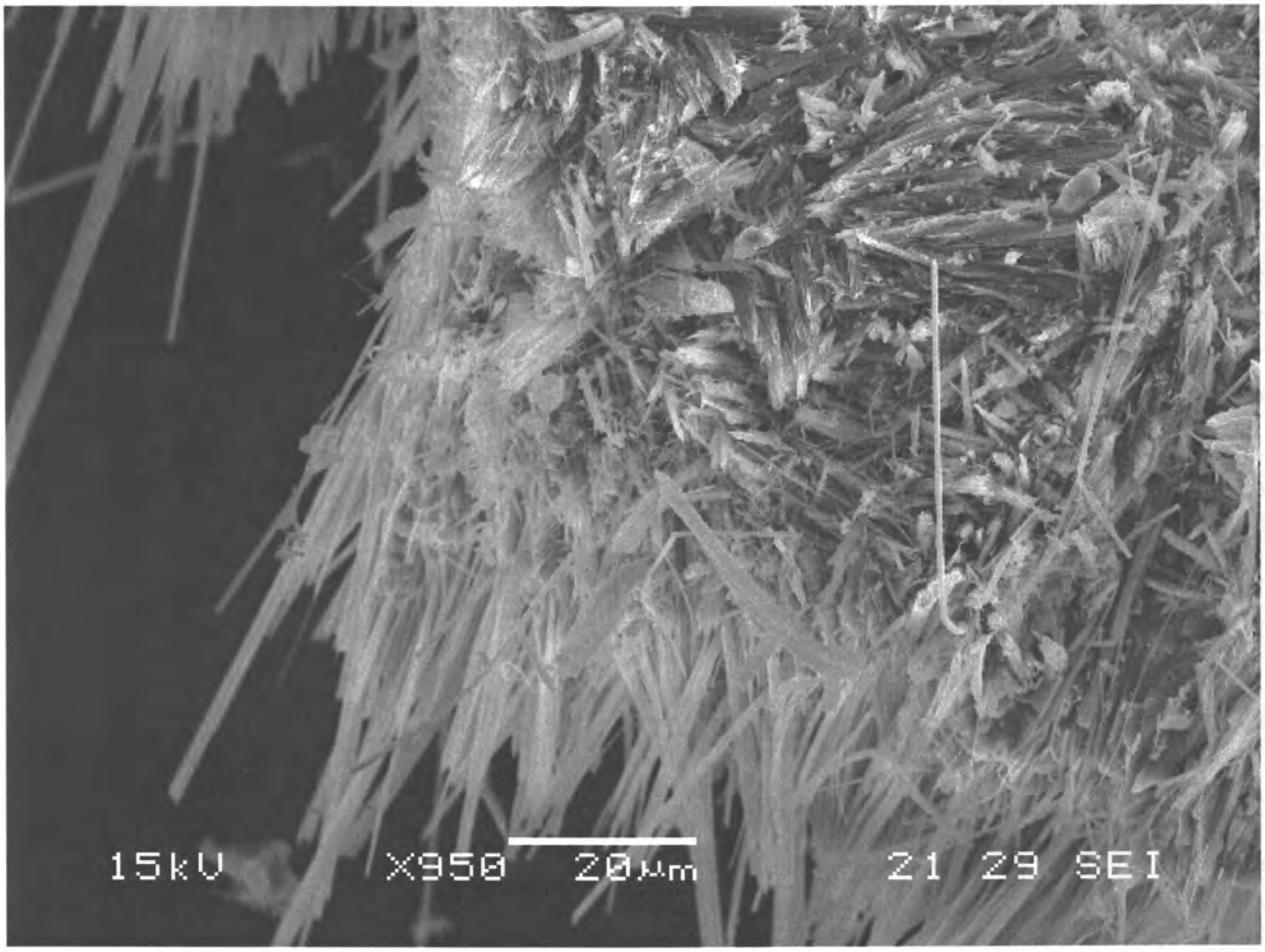


Figure 25. SEM image of a sample of series MgCl3M, as-received MgO particle after hydration in simplified GWB brine with MgO-to-brine ratio equal to 3 g/11 ml for 113 days. This image is recorded as H1I2.BMP in SN WIPP-MM MgO-7, pg. 57.

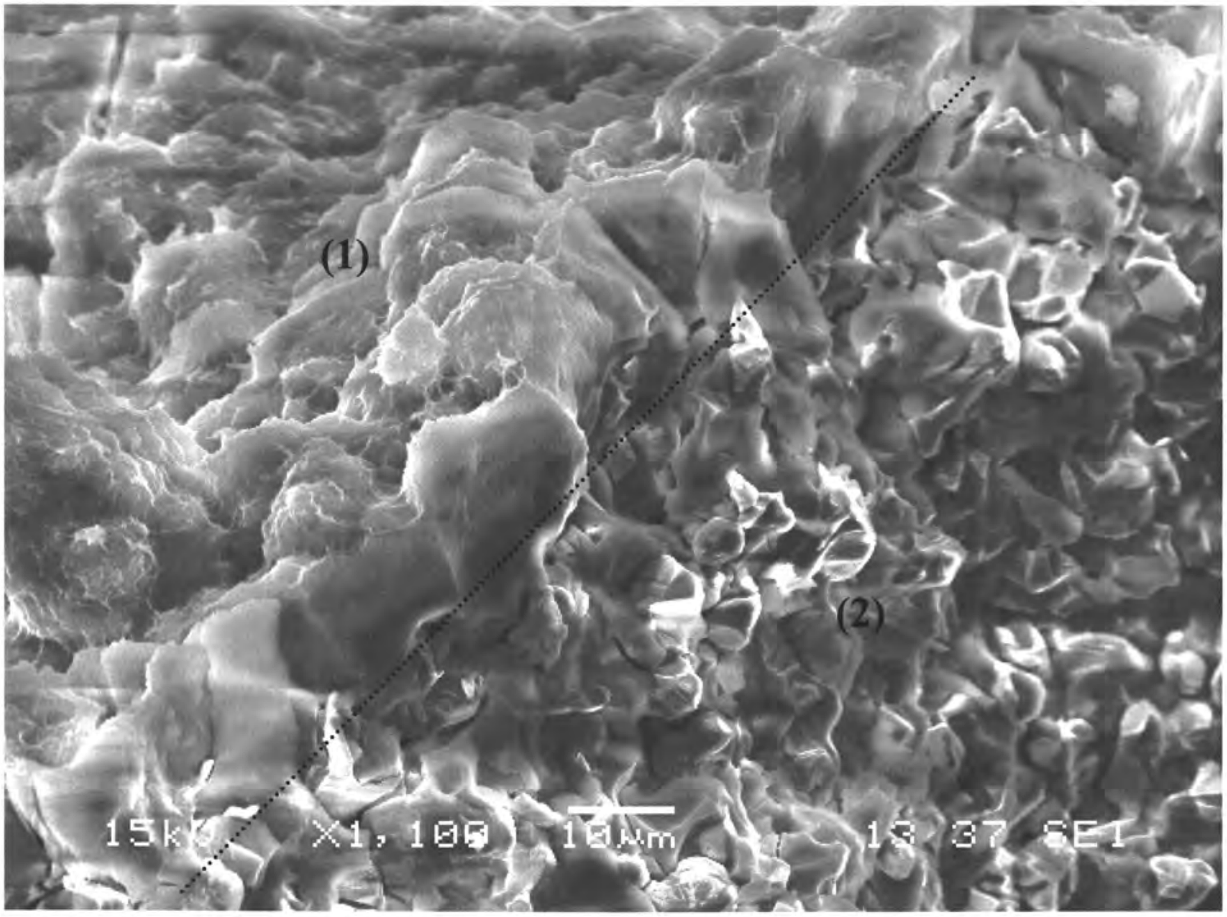


Figure 26. SEM image of a particle from series GW20L, large-MgO particles hydrated in GWB, with MgO-to-brine ratio equal to 3.1 g/77 ml, for 371 days. This image shows a particle that has been cut open using an exacto knife. Region 1 is on the exterior of the particle, region 2 is in the interior of the particle. A skin of hydration product (above the dotted lines) is visible of thickness around 10 μm. This image is recorded as H1I4B.BMP in SN WIPP-MM MgO-15, pg. 30.

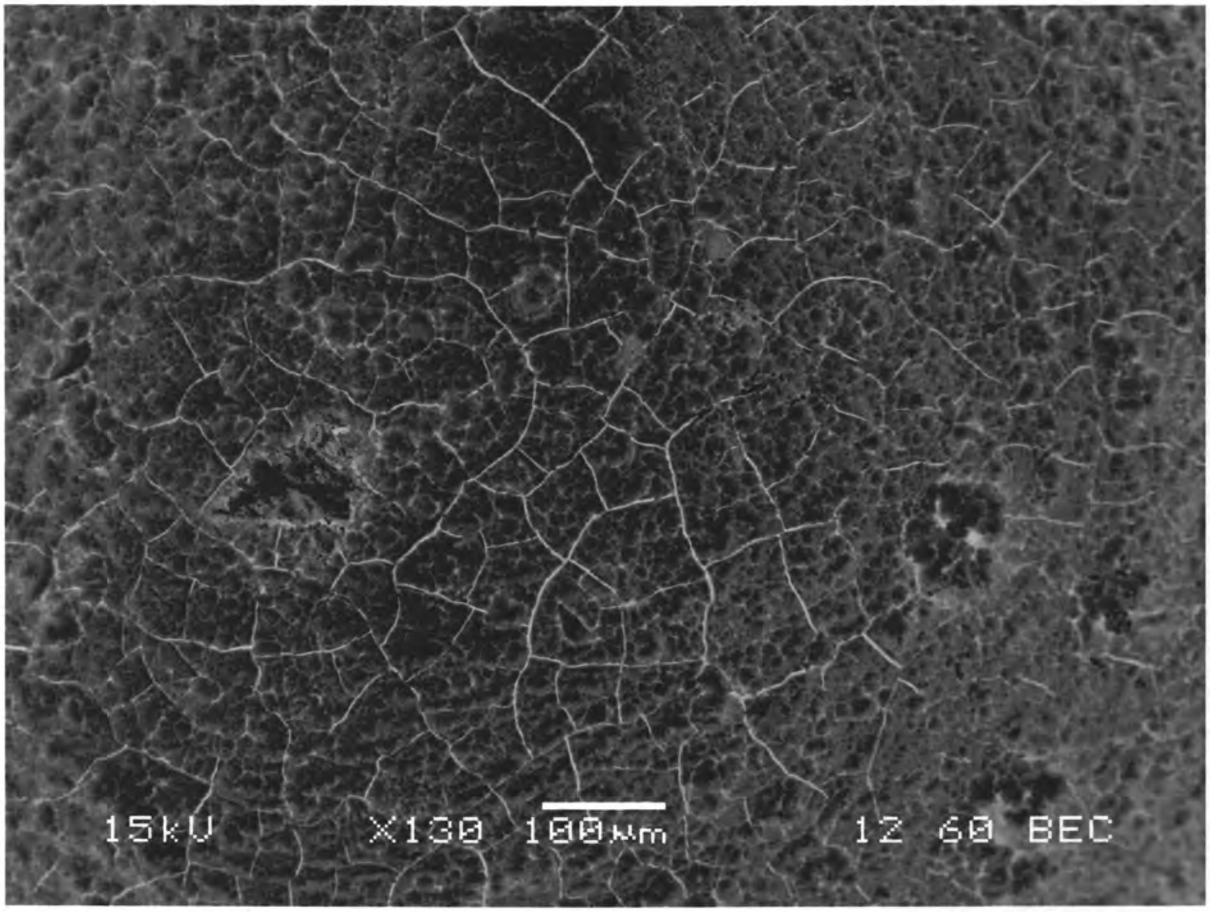


Figure 27. Back-scattered electron (BEC) image of the exterior of a particle from series GW20L, large MgO particles hydrated in GWB, with MgO-to-brine ratio equal to 3.1 g/77 ml for 371 days. A network of fractures (~1 μm aperture) is visible which will allow brine to further penetrate these particles. This image is recorded as H1I3.BMP in SN WIPP-MM MgO-15, pg. 30.

3.3 pH

The three brines used in the long-term hydration experiments are brines with high ionic strengths. In this report, we attempt to obtain hydrogen ion concentrations based on the pH reading and the correction factors calculated from Gran titrations of the brines. Rai et al. (1995) investigated the relationship between the log of hydrogen-ion concentration and pH measured by combination-glass electrode using Gran titrations. They reported a correction factor A for high-ionic-strength solutions containing NaCl or Na_2SO_4 or both,

$$pC_{H^+} = pH_{ob} + A, \qquad (1)$$

where pC_{H^+} is the negative log of hydrogen-ion concentration on a molarity scale and pH_{ob} is the observed pH reading of the brine using a combination-glass electrode. The constant A is then related to the activity of hydrogen by

$$A = \log \gamma_{H^+} + (F/2.303RT)/E_j, \qquad (2)$$

where γ_{H^+} is the molarity-scale activity coefficient of H^+ and E_j is the difference in liquid-junction potential between the low-ionic-strength standards and high-ionic-strength solutions.

Gran titrations can be performed using acid or base. Rai et al. (1995) reported that the correction factor A obtained by acid and base titration are consistent. Rai et al. (1995) also investigated the correction factor A of a limited number of Orion-Ross-glass-combination electrodes and found the value of A of different electrodes were close. Therefore, it may not be necessary to measure the correction factor A for every electrode.

Altmaier et al. (2003) determined the log of the hydrogen-ion concentration in a series of NaCl and $MgCl_2$ solutions by two methods. One method was Gran titrations using acid. The other was to measure the activity of HCl with a liquid-junction-free cell using a H^+ sensitive electrode and a chloride-sensitive electrode. They reported the hydrogen-ion concentration obtained from both methods were consistent within ± 0.04 log units, except for a 5.15m $MgCl_2$ solution.

We obtained the correction factor A for the three brines, GWB, ERDA-6, and simplified GWB by Gran titration using 1.00 M and 0.01 M HCl. The 1.00 M HCl was standardized against NaOH, which was first standardized by KHP (potassium hydrogen phalate). An Orion EA 940 pH/ion analyzer and two Ross electrodes were used to measure pH. The pH meter was calibrated by three pH buffers bracketing the sample pH range prior to measurement. In order to remove any dissolved carbon dioxide brine was purged by nitrogen for at least 5 minutes. Small amounts of HCl were delivered to the brine by an Eppendorf pipette. The observed pH values after each addition of HCl as well as the volume of HCl added to the brine were recorded in the scientific notebook. Since GWB and ERDA-6 contain small amounts of sulfate which can consume HCl to form bisulfate ions (HSO_4^-) at low pH,

$$HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}, \qquad (3)$$

the acid dissociation constant for reaction (3), K_a, was calculated by the FMT code (Babb and Novak, 1997). The values of Ka used and the FMT files from which they came are documented in Excel file "Brine acid base titration" on the worksheet "constant". Next the concentration of H^+ can be calculated from

$$H^+ = H^+_{add} /[1+ (1/K_a) [SO_4^{2-}]], \tag{4}$$

where $[SO_4^{2-}]$ is the molar concentration of sulfate. Next, plots of the observed $[H_{ob}^+]$ (equal to 10^{-pH}) versus H^+ obtained by equation (4) were prepared. The correction factor A was then obtained by taking the log of the slope of these plots.

The correction factors A for ERDA-6, GWB, and simplified GWB are 1.155, 1.236, and 1.202 respectively. The detailed calculation for these correction factors is located in Excel file "Brine Acid Base Titration"; see the worksheet "sum" for a summary of these calculations. Using the obtained correction factors for GWB, simplified GWB and ERDA-6, the brine pmH (-log m_H^+) are shown in section 4.4.

4 THERMODYNAMICS

4.1 Discussion of phase 3 and phase 5

Sorel first reported making a cementitious material by mixing calcinated magnesia with concentrated magnesium chloride solution in 1867 (Sorel, 1867). Such material has been referred to as Sorel cement, magnesia cement, or magnesium-oxychloride cement. Magnesium-oxychloride cement (MOC) is now the generally used term. MOC has been an important building material by virtue of its high fire resistance, low thermal conductivity and marble-like appearance. Various forms of magnesium oxychloride have been identified in the system of MgO-$MgCl_2$-H_2O and $NaOH$-$MgCl_2$-H_2O. Designated by the number of moles of OH appearing in its formula in relation to that of Cl, they are, $Mg_3(OH)_4Cl_2{\cdot}2H_2O$ (phase-2), $Mg_2(OH)_3Cl{\cdot}4H_2O$ (phase-3), $Mg_3(OH)_5Cl{\cdot}4H_2O$ (phase-5), and $Mg_5(OH)_9Cl{\cdot}5/2H_2O$ (phase-9). Some researchers give a different formula for phase-9, $Mg_5(OH)_9Cl$ $1/2H_2O$ (Maravelaki-Kalaitzaki and Moraitou, 1999). Only phase-3 and phase-5 have been found to form at ambient temperatures (Demediuk et al., 1955; Newman, 1955; Matkovic et al., 1977; Mazuranic et al., 1982; Bilinski et al., 1984), and thus are of particular interest to us. Previous research on Premier-MgO hydration found the formation of brucite from MgO hydrated in ERDA-6, and formation of phase-5 and brucite in GWB brine (Xiong and Snider Lord, 2008). Brucite has also been proposed to be added to the Asse salt mine in Germany (Altmaier et al., 2003). Phase-3 and brucite formation have been observed in Asse-relevant brines. These phases may have an important effect on pH, thereby affecting actinide solubilities in brine.

A. The formation of magnesium oxychloride

The crystallization of a particular MOC phase depends on the total amount of Mg and Cl and the pH of the solution (Demediuk et al., 1955; Mazuranic et al., 1982; Bilinski et al., 1984). Demediuk et al. (1955) studied the MgO-$MgCl_2$-H_2O system at temperatures between 0 and 110 °C. They added 0.4 g of MgO to 20 ml of $MgCl_2$ solution at various concentrations between 10 and 40 w/v % (1.13 – 4.74 m). According to their results, at temperatures around 30 °C, a mixture of phase-5 and brucite formed at $MgCl_2$ concentrations lower than 18 % w/v (1.99 m), while phase-5 alone formed in $MgCl_2$ solutions of 23 % w/v (2.67 m). At $MgCl_2$ solution concentrations of 30 % w/v (3.49 m), phase-3 was precipitated. Mazuranic et al. (1982) studied the system of $NaOH$-$MgCl_2$-H_2O. NaOH was added to $MgCl_2$ solutions of 0.001- 4.8M (0.001 – 5.68 m). Phase-3 and phase-5 formed only in mixtures that had a $MgCl_2$ concentration greater than 1.96 M. Altmaier (2003) studied the solubility of $Mg(OH)_2$ in water, 0.01-2.7 m $MgCl_2$, 0.1-5.6 m NaCl and in mixtures of 0.5 and 5.0 m NaCl containing 0.01-0.05 m $MgCl_2$. It was found that the $Mg(OH)_2$ completely converted into phase-3 in $MgCl_2$ solutions above 2 molal. In $MgCl_2$ solutions of 2.67 m and 5.15 m, the pH decreased 0.2-0.5 units, as a result of the phase change.

B. The reaction of phase 3 and phase 5[c1] with water and carbon dioxide

On continued exposure to water, MOC hydrolyzes slowly and magnesium chloride is leached out (Maravelaki-Kalaitzaki and Moraitou, 1999). de Castellar et al. (1996) showed that a polished MOC brick cracks after five months due to the formation of oxychloride-carbonate

($Mg(OH)_2 \cdot 2\ MgCO_3 \cdot MgCl_2 \cdot 6H_2O$) produced from phase-3 carbonation. In a 22-yr-old specimen which was temporarily exposed to rain, hydromagnesite was the predominant phase on the surface with phase-5, brucite, and oxychloride-carbonate present in the interior of the specimen (Matkovic et al., 1977). Maravelaki-kalaitzaki (1999) and Demediuk (1955) also found oxychloride-carbonate in Sorel's cement containing phase-3 and phase-5. The formation of the oxychloride-carbonate is temperature and humidity-dependent and is favored at relative humidity greater than 60% (Maravelaki-Kalaitzaki and Moraitou, 1999). Further carbonation of oxychloride-carbonate generates hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$) (Maravelaki-Kalaitzaki and Moraitou, 1999).

C Quantification of the weight fractions of phase 3 and phase 5

Powder X-ray diffraction (XRD), SEM, EDS, FT-IR and differential thermal analysis have been used by researchers to identify the presence of phase-3 and phase-5. However, quantitative analysis of phase-3 and phase-5 is difficult. Most researchers use semi-quantitative methods to determine the amount of phase-3/5 by XRD (Bilinski et al., 1984). Others use chemical analysis (Demediuk et al., 1955) to quantify the amount of MgO and chloride, using toxic chemicals such as Hg_2O. TGA and DSC are not viable methods because phase-3 loses water at 100-250 and 300-500 °C, and phase-5 loses water at 70-250, 300-500 °C. Thus both phase-5 and phase-3 decompositions overlap with the water-loss of brucite at 350-500 °C, which makes it impossible to quantitatively determine the amount of phase-3, phase-5 and brucite using TGA or DSC (Demediuk et al., 1955) . As discussed in Section 3.1, in future work we will use XRD and the Rietveld method to quantify the weight percent of mineral phases.

4.2 Saturation index of phase 5, phase 3 and brucite

In section 3.1 it was shown that MgO hydrated in ERDA-6 produces brucite, and MgO hydrated in simplified GWB or GWB produces phase-5 and brucite. Next we present the experimental saturation index (SI) of phase 5, phase 3 and brucite versus time in the three brines. SI is defined as

$$SI = \log(Q/K) \qquad (5)$$

where Q is the ion activity product and K is the equilibrium constant of a given phase. When SI > 0, the solution is over-saturated with respect to the phase, i.e. the solid phase is forming. When SI < 0, the solution is under-saturated with respect to that phase. We calculated log Q for phase-5, phase-3 and brucite according to the following equations:

phase-5:

$$Mg_3Cl(OH)_5 \bullet 4H_2O + 5H^+ = 3Mg^{2+} + 9H_2O(l) + Cl^-$$

$$\log Q\ (\text{phase-5}) = 3 \log (m_{mg^{2+}}\ \gamma_{mg^{2+}}) + \log (m_{Cl^-}\ \gamma_{Cl^+}) - 5 \log(m_{H^+}\ \gamma_{H^+}) + 9 \log a_w \qquad (6)$$

phase-3:

$$Mg_2Cl(OH)_3{\bullet}4H_2O + 3H^+ = 2Mg^{2+} + 7H_2O(l) + Cl^-$$

$$\log Q \text{ (phase-3)} = 2 \log (m_{mg}{}^{2+} \gamma^-_{mg}{}^{2+}) + \log (m_{Cl^-} \gamma_{Cl}{}^+) - 3 \log (m_H{}^+ \gamma_H{}^+) + 7 \log a_w \qquad (7)$$

brucite:

$$Mg(OH)_2 + 2H^+ = Mg^{2+} + 2H_2O(l)$$

$$\log Q \text{ (brucite)} = \log (m_{mg}{}^{2+} \gamma^-_{mg}{}^{2+}) - 2 \log(m_H{}^+ \gamma_H{}^+) + 2 \log a_w \qquad (8)$$

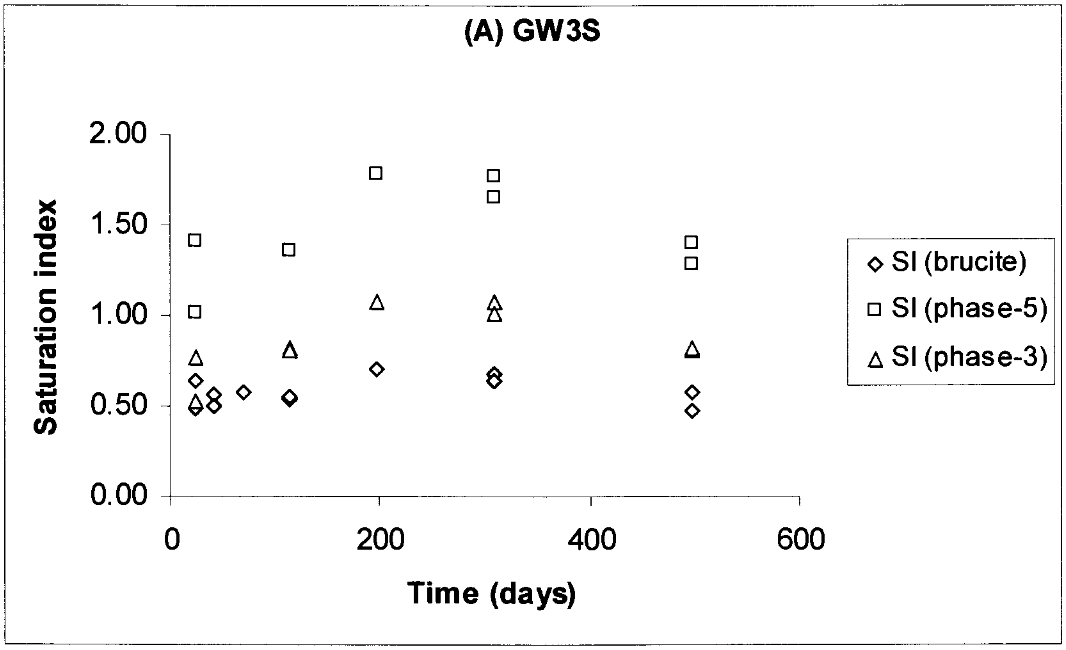
In equations (6) - (8), $m_{mg}{}^{2+}$, $m_{Cl}{}^-$ and $m_H{}^+$ are the molal concentrations of Mg^{2+}, Cl^- and H^+ which were determined experimentally (see experimental section). Using the database "data1.ph5" the activity coefficients $\gamma_{Mg}{}^{2+}$, $\gamma_{Cl}{}^-$, $\gamma_H{}^+$ and the water activity a_W were obtained from EQ3/6 runs simulating the reaction path way of periclase being titrated into a closed system containing one of the three brines (ERDA-6, GWB, simplified GWB). Database "data1.ph5" has been modified from "data0.hmo" by adding the solubility constant for phase-5 (Xiong et al, 2009) calculated from the specific interaction model (SIT).

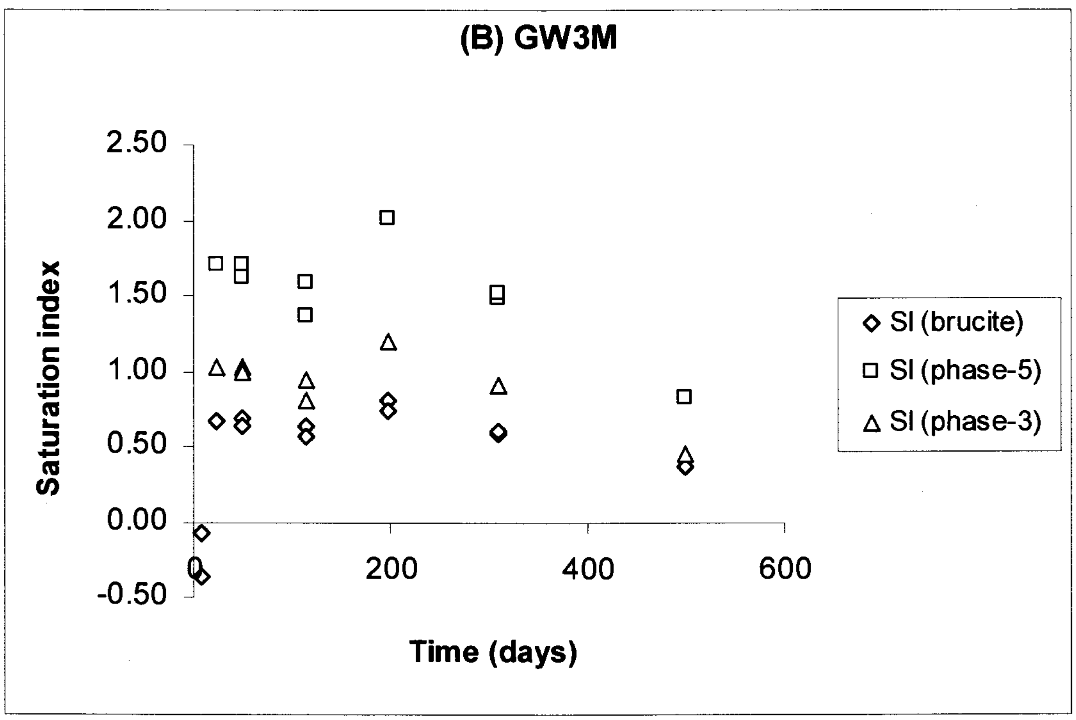
We also calculated the solubility constant of phase-5 using EQ3/6. This was accomplished by entering the experimentally measured magnesium, and chloride concentrations, setting the sodium concentration to achieve charge balance, and adjusting the log K of phase-5 until the predicted pmH matched the experimentally determined value (a manual optimization technique). While this method is self consistent with the rest of EQ3/6 calculations reported in this document, the difference between the log K (phase-5) using this method and the SIT method is only 0.2 log units, which is within experimental error (2σ). This work was performed under AP-108. This work is a deviation from that analysis plan where no EQ3/6 or FMT runs were originally planned.

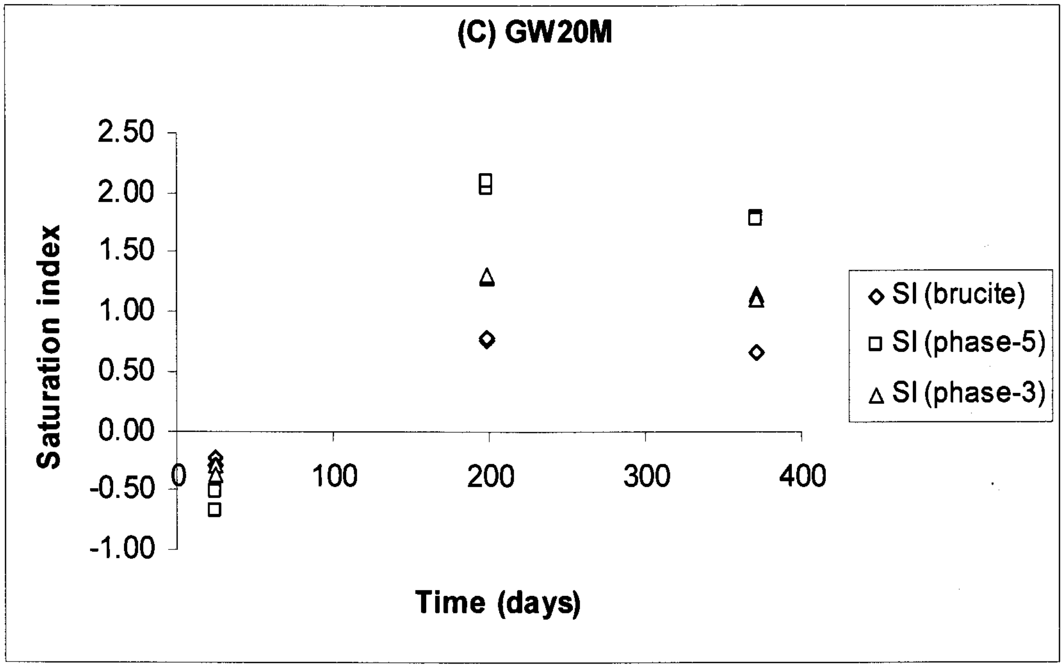
Various solubility constants for brucite and phase-3 are available in the literature. Altmaier et al. (2003) determined the log K for brucite at 22 °C from solubility experiments with brucite in 0.01 - 2.7 m $MgCl_2$, 0.1 - 5.6 m NaCl, and mixtures of $MgCl_2$ and NaCl solutions. They also obtained the log K for phase-3, by performing solubility experiments in 2.11-5.15 m $MgCl_2$ solutions. Both values, $\log K_{brucite} = 17.1$ and $\log K_{phase\text{-}3} = 26.0$ are slightly different from the value used in our calculation, when they are extrapolated to the reference temperature 25 °C. Xiong (2008) recommended a solubility constant value for brucite based on experiments from supersaturation and undersaturation, $\log K_{brucite} = 17.05$ at 25 °C. The solubility constants for brucite and phase-3 used in this report are taken from the EQ3/6 database "data0.hmo", $\log K_{brucite} = 17.1090$, $\log K_{phase\text{-}3} = 26.0297$. The solubility constant for phase-5 used in this report, $\log K_{phase\text{-}5} = 43.17$, is taken from Xiong et al. (2009).

Figure 28 - Figure 29 show the SI for phase-5, phase-3 and brucite from hydration experiments conducted in GWB and simplified GWB. In general, the SI for all three phases are over-saturated or near equilibrium in GWB and simplified GWB. However, we did not observe phase-3 in any of the XRD files. The stability diagrams of the three phases presented in the next section may explain why phase-5 formed instead of phase-3. Detailed calculations for the

saturation index presented in Figure 28 - Figure 29 can be found in Excel file “Plots” worksheet “Fig 28’and “Fig 29”.


(A) GW3S
Saturation index
2.00
1.50
1.00
0.50
0.00
0
200
400
600
Time (days)
SI (brucite)
SI (phase-5)
SI (phase-3)


(B) GW3M
Saturation index
2.50
2.00
1.50
1.00
0.50
0.00
-0.50
0
200
400
600
Time (days)
SI (brucite)
SI (phase-5)
SI (phase-3)



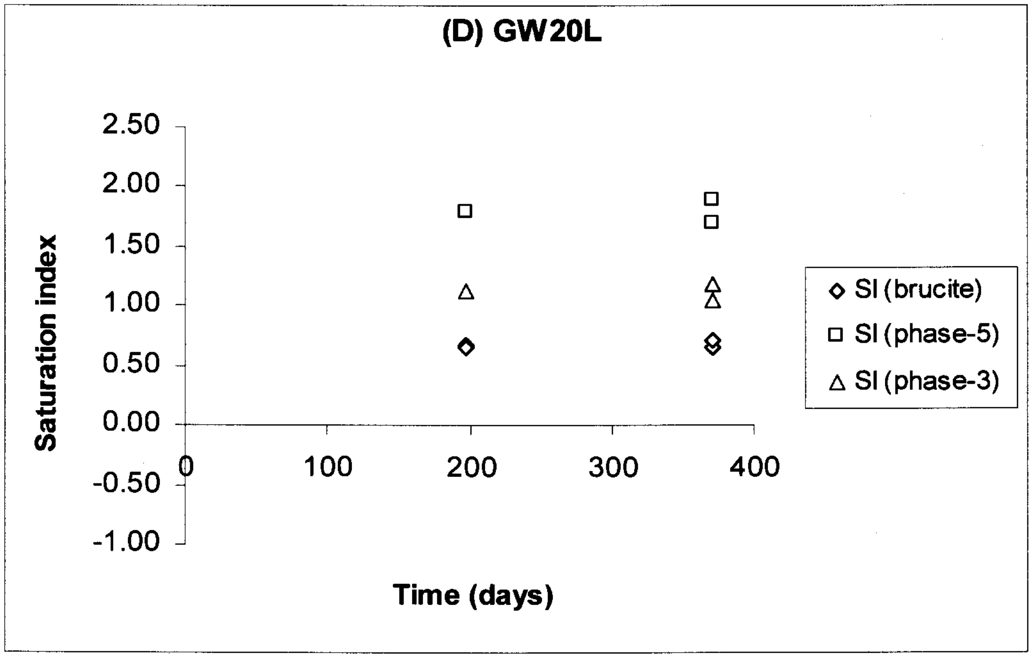
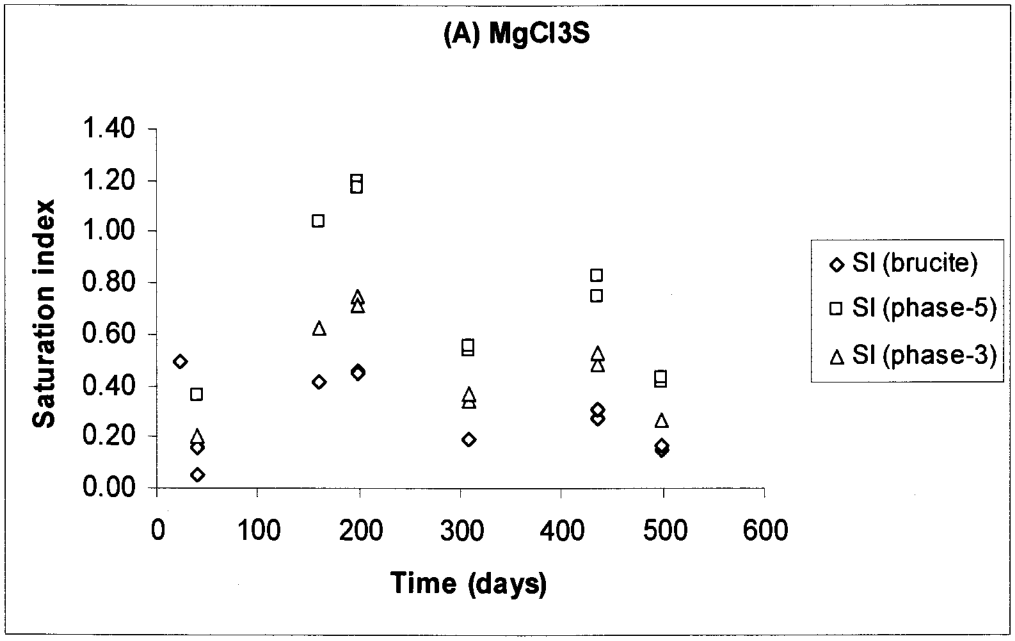
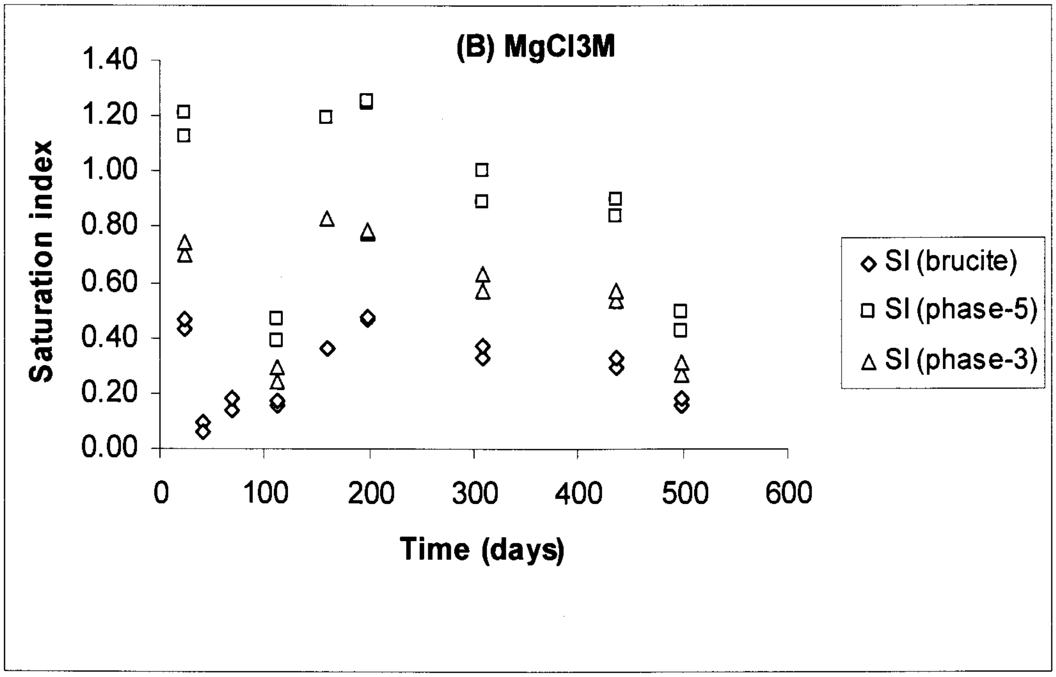
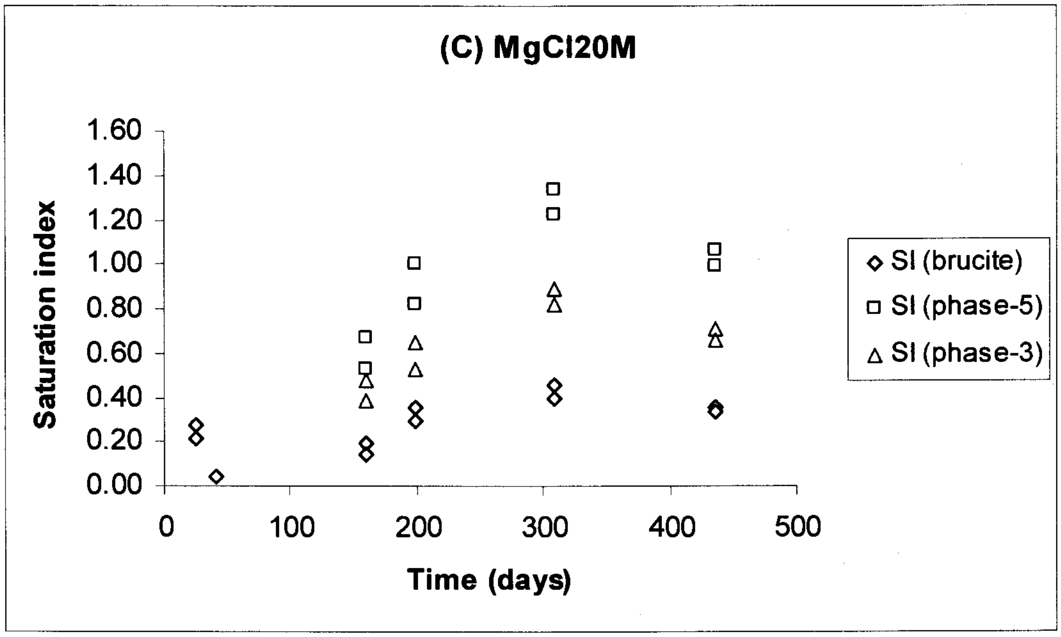


Figure 28 (A-D). Saturation index (SI) of brucite, phase-5, and phase-3 for MgO hydrated in GWB brine. See Table 1 for description of each experimental GW series.


(A) MgCl3S
Saturation index
Time (days)
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0
100
200
300
400
500
600
SI (brucite)
SI (phase-5)
SI (phase-3)


(B) MgCl3M
Saturation index
Time (days)
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0
100
200
300
400
500
600
SI (brucite)
SI (phase-5)
SI (phase-3)



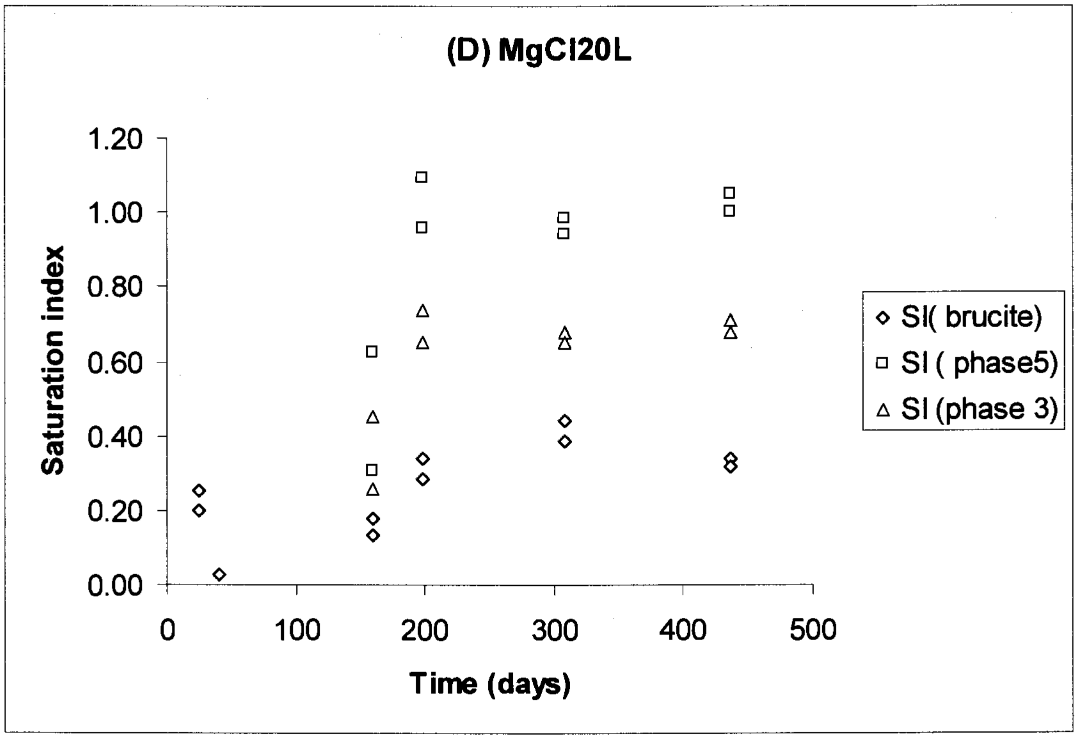


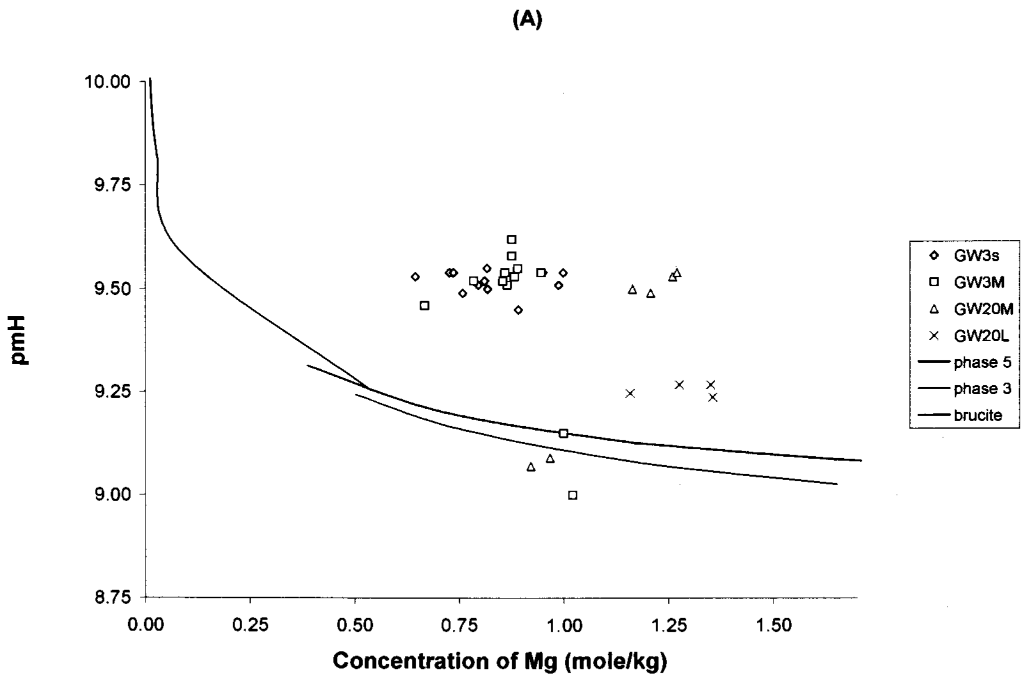
Figure 29 (A-D). Saturation index of brucite, phase-5, and phase-3 for MgO hydrated in simplified GWB brine. See Table 1 for description of each experimental simplified GWB series.

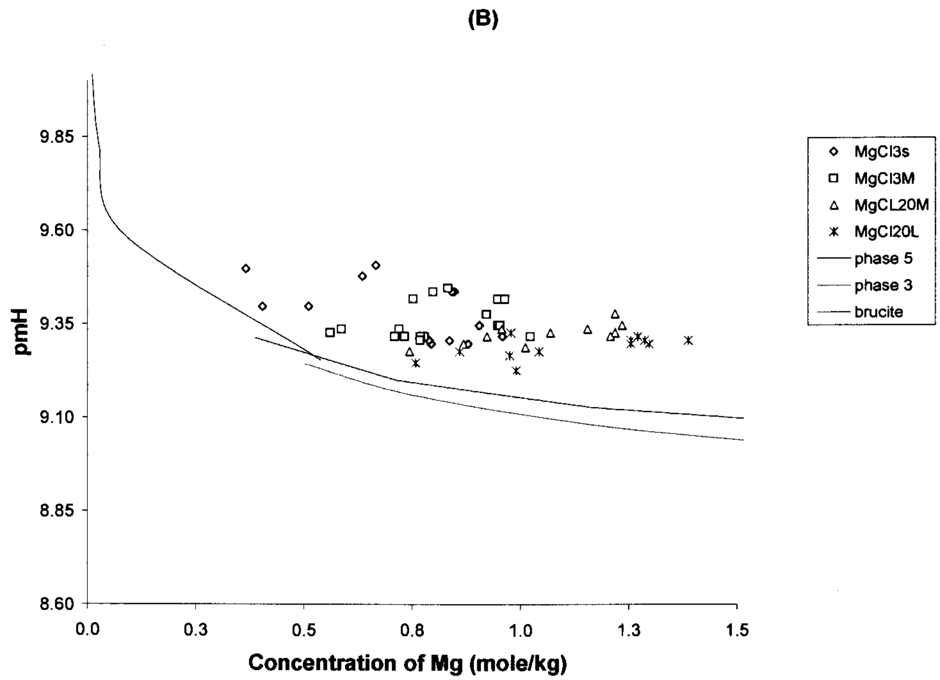
4.3 Relative stability of phase 5, phase 3 and brucite

The saturation indices given in section 4.2 indicate that phase-5, phase-3 and brucite are near or over-saturated in GWB and simplified GWB. However, as shown by XRD in section 3.1, MgO hydrated in ERDA-6 produces brucite, and MgO hydrated in simplified GWB or GWB produces phase-5 in addition to brucite. This can be understood by plotting the experimental data on phase diagrams for phase-5, phase-3 and brucite. Figure 30 shows the pmH of phase-5, phase-3, and brucite versus $m_{Mg}{}^{2+}$ calculated using EQ3/6 (Xiong et al, 2009) and the experimental data points from the three brines. Figure 30 can be interpreted as a stability-field diagram for the three phases.

As shown in Figure 30, for a given molality of Mg^{2+}, phase-5 is a stable phase at higher pmH, and phase-3 is a stable phase at lower pmH. Brucite is the stable phase in a solution with a low Mg^{2+} concentration and high pmH. In solutions typical of GWB, the separation between the stability field of phase-5 and that of phase-3 is narrow for low Mg^{2+} concentrations (e.g., 0.5 m of Mg^{2+}), but the separation widens as the Mg^{2+} concentration increases. Therefore, the stability fields of phase-5 and phase-3 could be considered to be overlapping in the range of low Mg^{2+} concentration when the uncertainty in the thermodynamic data is taken into account. However, in the range of high Mg^{2+} concentrations, these two phases have their respective well-defined fields. Our experimental data (>80%) are overwhelmingly in the stability field of phase-5 (Figures 30A-B), which is in excellent agreement with our laboratory observations (see Section 3.1).

In solutions typical of ERDA-6, which have Mg^{2+} concentrations lower than 0.2 m, the separation among the stability fields of brucite, phase-5, and phase-3 is small (Figure 30C). Therefore, brucite is the stable phase because of its lower solubility. The majority of our experimental data falls into the stability field of brucite, which is in agreement with our laboratory observations that only brucite is formed in experiments with ERDA-6.


(A)
10.00
9.75
9.50
9.25
9.00
8.75
pmH
0.00
0.25
0.50
0.75
1.00
1.25
1.50
Concentration of Mg (mole/kg)
GW3s
GW3M
GW20M
GW20L
phase 5
phase 3
brucite


(B)
9.85
9.60
9.35
9.10
8.85
8.60
pmH
0.0
0.3
0.5
0.8
1.0
1.3
1.5
Concentration of Mg (mole/kg)
MgCl3s
MgCl3M
MgCL20M
MgCl20L
phase 5
phase 3
brucite

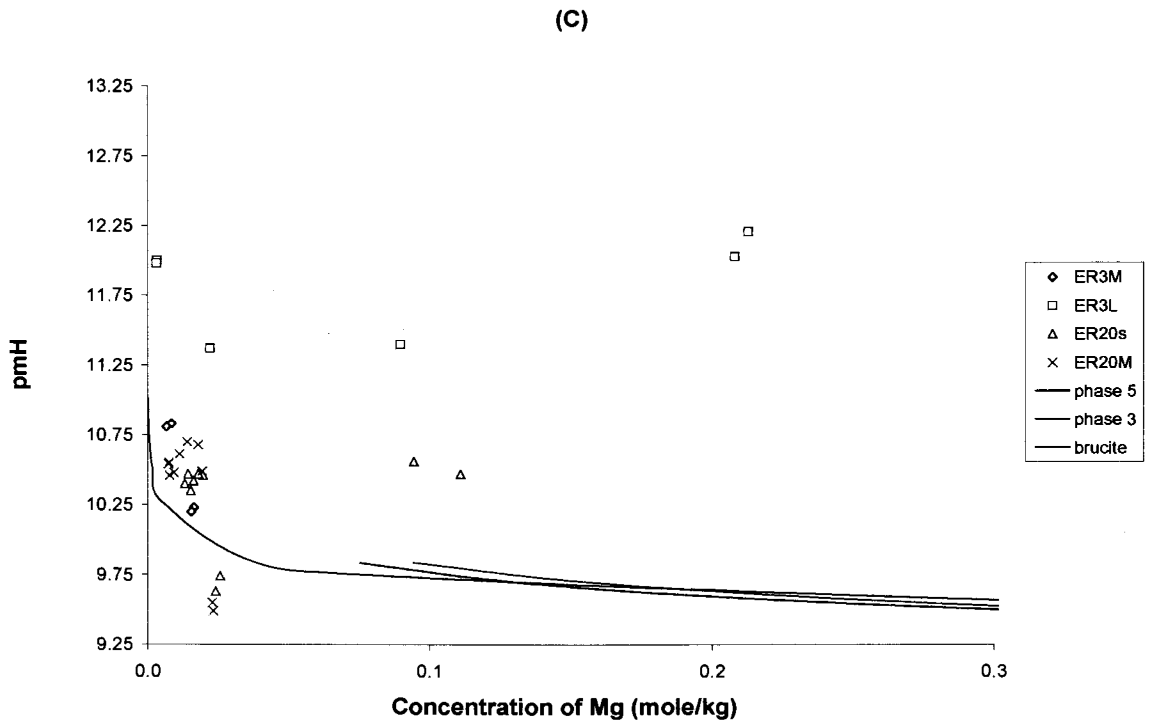


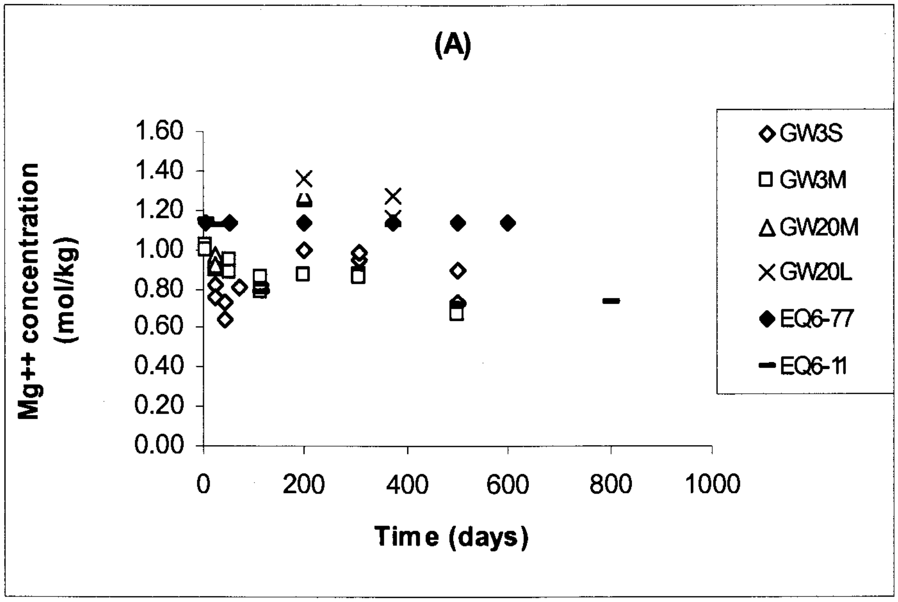
Figure 30 (A-C). Phase diagrams for phase-5, phase-3 and brucite in various brines. Plots (A) and (B) have NaCl and $MgCl_2$ concentrations characteristic of GWB and simplified GWB. Plot (C) has NaCl and $MgCl_2$ concentrations characteristic of ERDA-6. All lines were calculated using EQ3/6 (Xiong et al, 2009). The symbols represent experimental data points.

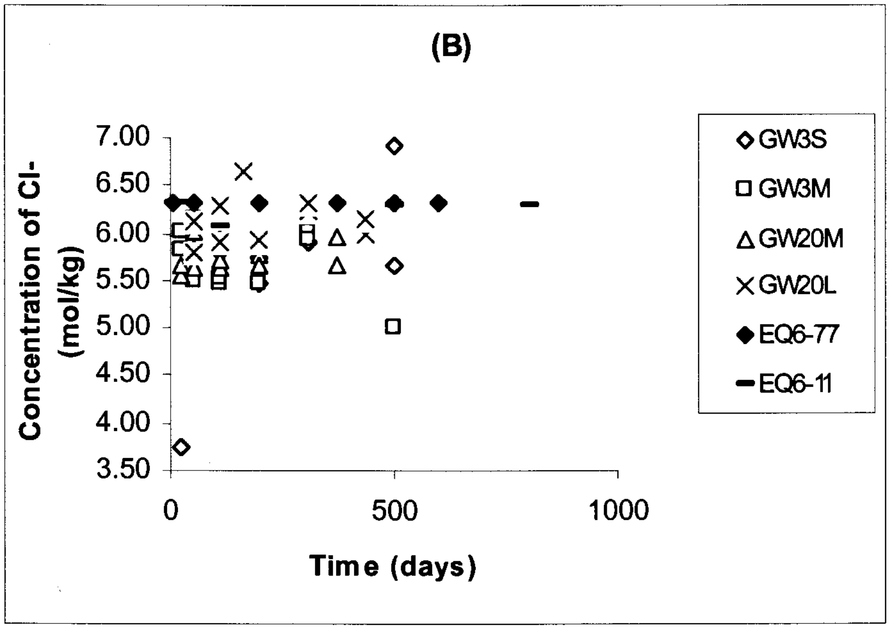
4.4 Brine Chemistry

We used EQ3/6 to simulate the reaction path way of MgO hydration and carbonation in a closed system containing brine and atmospheric carbon dioxide by titrating periclase into the system. The amount of periclase titrated into GWB and ERDA-6 brine was calculated from the brine density (the brine recipe is given in SP 20-4) and the experimental brine-to-MgO ratios. The amount of periclase titrated into simplified GWB was similarly calculated, except the density of simplified GWB was measured (documented in scientific notebook WIPP-CBD-26, p82). In the simulations of MgO hydrated in ERDA-6, we also added portlandite to generate pH values and Ca concentrations similar to the experimentally observed values. In the model, portlandite was added before periclase was added, as lime hydrates much faster than periclase. The amount of portlandite added was calculated based on the mole ratio of periclase to lime reported by Deng et al. (2008). We did not add portlandite into GWB or simplified GWB because the high concentration of Mg in these brines will buffer pH. In addition, we suppressed the formation of phase-3 in our model as phase-3 was never observed in the hydration products. Detailed calculations of the amount of periclase and lime used in the EQ3/6 simulations can be found in the Excel file “MgO in brine”.

The EQ3/6 model predicted the formation of brucite in ERDA-6 brine, and the formation of brucite and phase-5 in GWB and simplified GWB with MgO-to-brine ratio equal to 3 g/11 ml, which is consistent with our experiments. The EQ3/6 model also predicted the formation of phase-5 in GWB with a MgO-to-brine ratio equal to 3.1 g/77 ml, which is consistent with our experiments. The model did not predict brucite formation in simplified GWB with MgO-to-brine ratio equal to 3.1 g/77 ml, which is not consistent with our experiments. According to the model, when periclase is titrated into the GWB or simplified GWB, phase-5 forms as the Mg/Cl concentrations decrease and pH increases until certain points, where brucite starts to precipitate out with phase-5. From the EQ3/6 runs, brucite is predicted to form in simplified GWB when the Mg concentration < 0.70 m, Cl concentration <5.98 m and pmH ≥ 9.25. In GWB, brucite is predicted to form when the Mg concentration < 0.78 m, Cl concentration <6.08 m, and pmH ≥ 9.26. The EQ3/6 run execution information can be found in appendix A. A summary of results from the EQ3/6 runs is available in Excel file "Plots" worksheet "Fig 31' "Fig 32", and "Fig 33", in addition to the original EQ3/6 input / output files.

Figure 31 - Figure 33 compare the measured Mg concentration, Cl concentration, pmH with EQ6 predicated values. In these figures, EQ6-77 and EQ6-11 represent reaction pathway of MgO hydrated in 77 ml and 11ml brine with arbitrary time scaling.


(A)
Mg++ concentration (mol/kg)
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0
200
400
600
800
1000
Time (days)
GW3S
GW3M
GW20M
GW20L
EQ6-77
EQ6-11


(B)
Concentration of Cl- (mol/kg)
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
0
500
1000
Time (days)
GW3S
GW3M
GW20M
GW20L
EQ6-77
EQ6-11

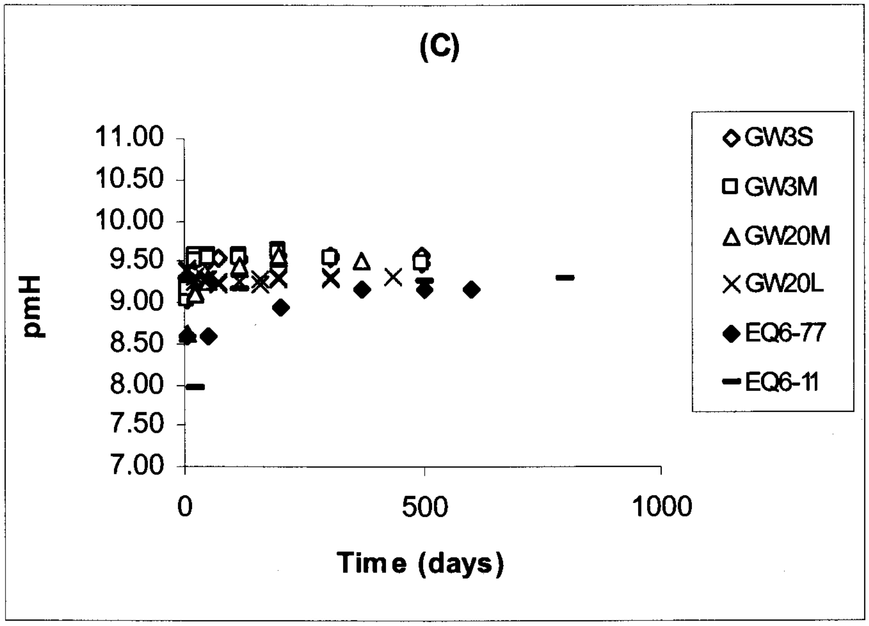
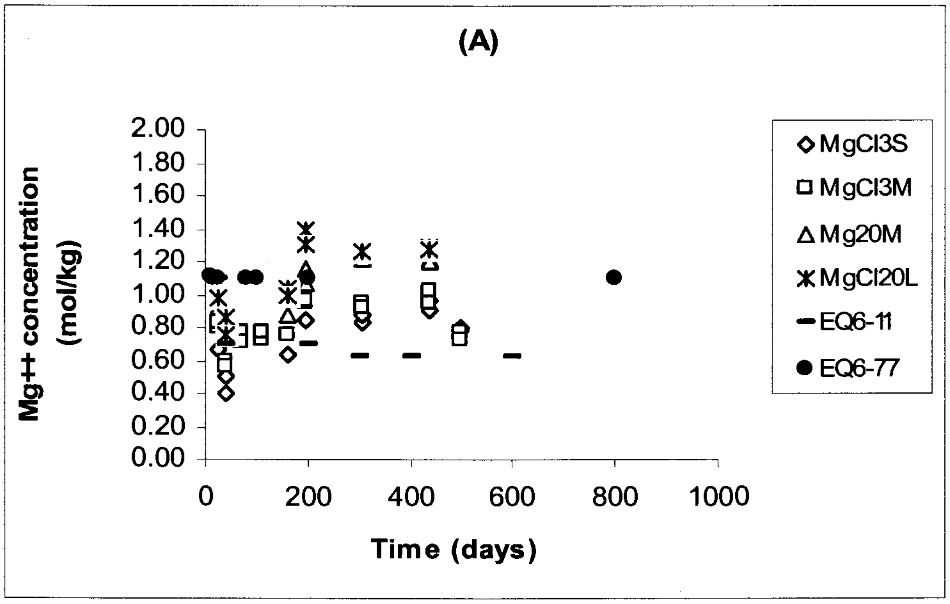
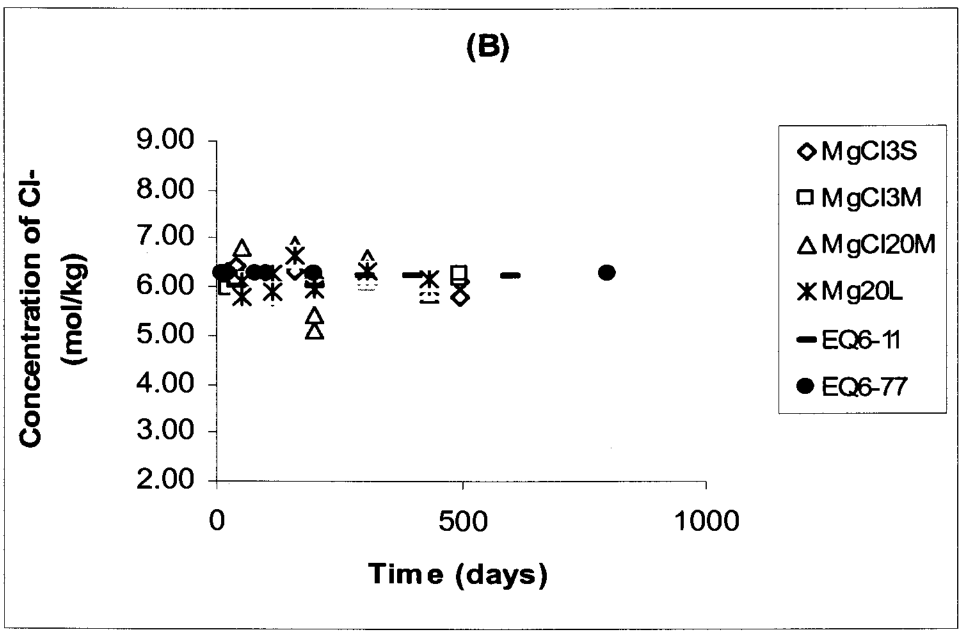


Figure 31. Plots showing experimental concentrations of (A) Mg^{2+}, (B) Cl^-, and (C) pmH versus time (days) for MM MgO hydrated in GWB, and the results of the EQ3/6 modeling runs titrating periclase into GWB brine. The experimental conditions corresponding to each GW series can be found in Table 1. The series EQ6-77 and EQ6-11 represent the EQ3/6 modeling runs of MgO hydrated in 77 ml and 11ml brine with arbitrary time scaling.


(A)
Mg++ concentration (mol/kg)
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0
200
400
600
800
1000
Time (days)
MgCl3S
MgCl3M
Mg20M
MgCl20L
EQ6-11
EQ6-77


(B)
Concentration of Cl- (mol/kg)
9.00
8.00
7.00
6.00
5.00
4.00
3.00
2.00
0
500
1000
Time (days)
MgCl3S
MgCl3M
MgCl20M
Mg20L
EQ6-11
EQ6-77

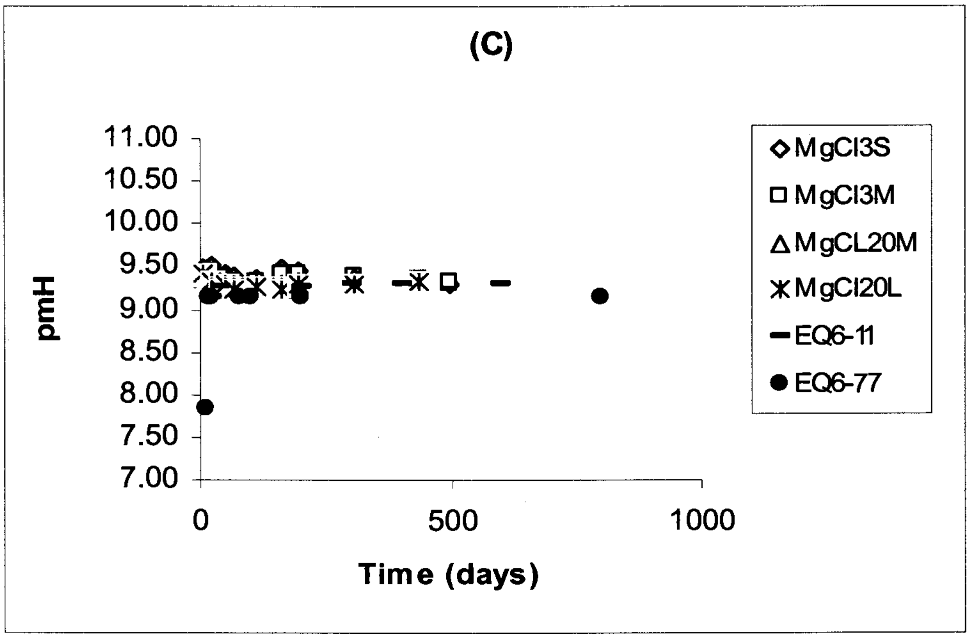
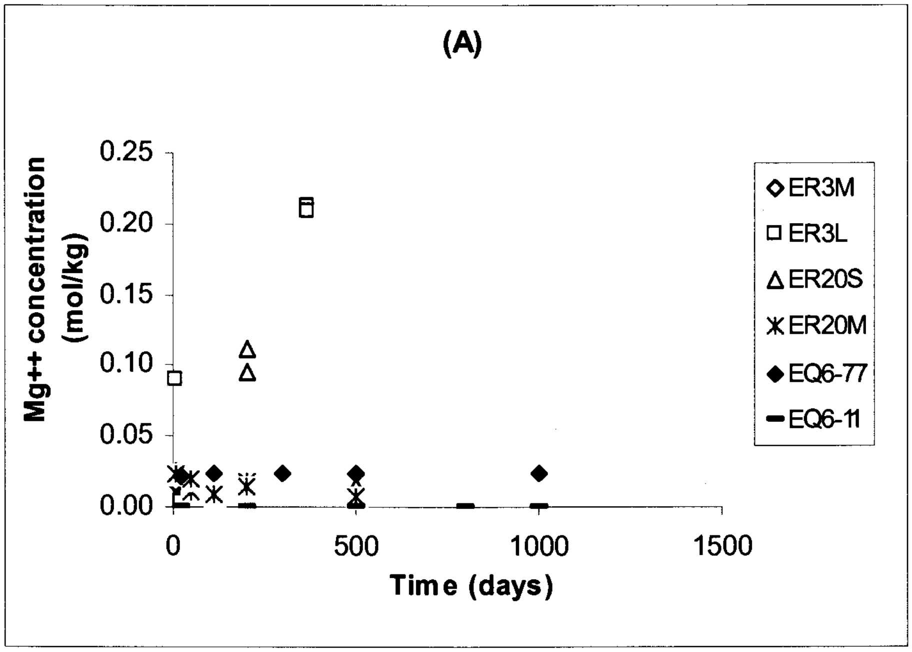
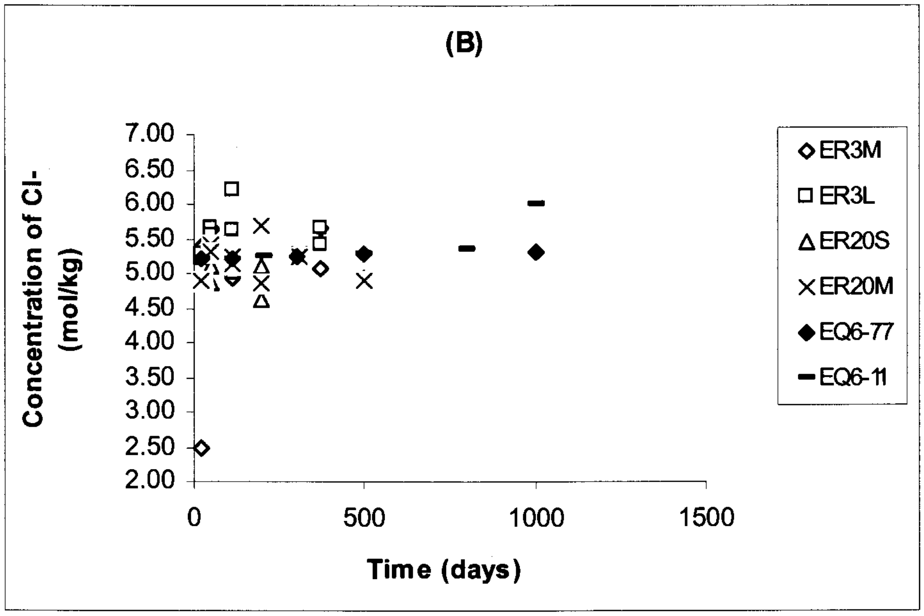
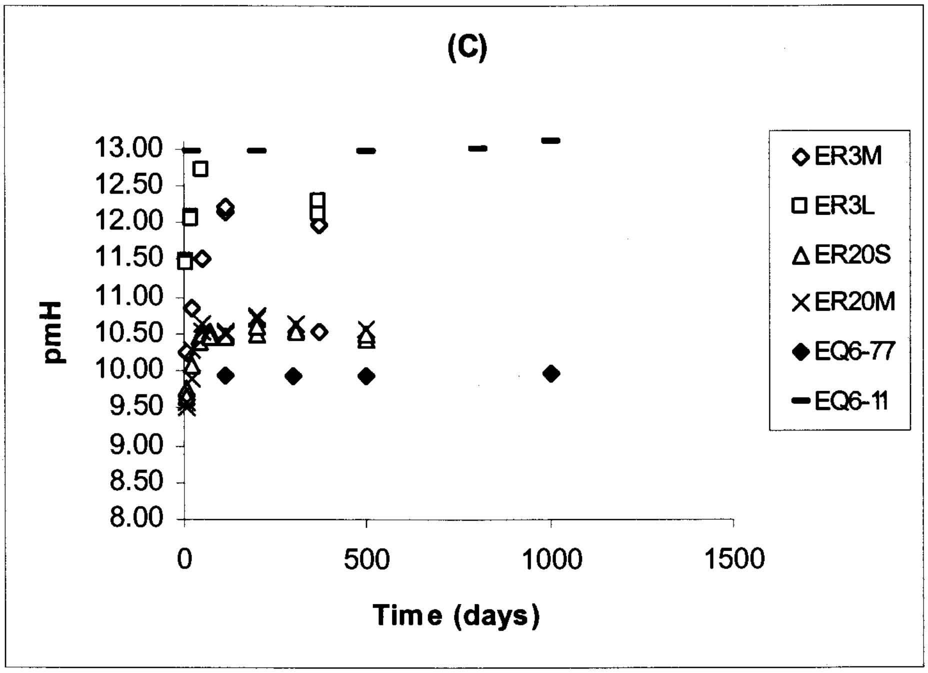


Figure 32. Plots showing experimental concentrations of (A) Mg^{2+}, (B) Cl^{-}, and (C) pmH versus time (days) for MM MgO hydrated in simplified GWB, and the results of the EQ3/6 modeling runs titrating periclase into simplified GWB brine. The experimental conditions corresponding to each MgCl series can be found in Table 1. The series EQ6-77 and EQ6-11 represent the EQ3/6 modeling runs of MgO hydrated in 77 ml and 11ml brine with arbitrary time scaling.


(A)
Mg++ concentration (mol/kg)
0.25
0.20
0.15
0.10
0.05
0.00
0
500
1000
1500
Time (days)
ER3M
ER3L
ER20S
ER20M
EQ6-77
EQ6-11


(B)
Concentration of Cl- (mol/kg)
7.00
6.50
6.00
5.50
5.00
4.50
4.00
3.50
3.00
2.50
2.00
0
500
1000
1500
Time (days)
ER3M
ER3L
ER20S
ER20M
EQ6-77
EQ6-11



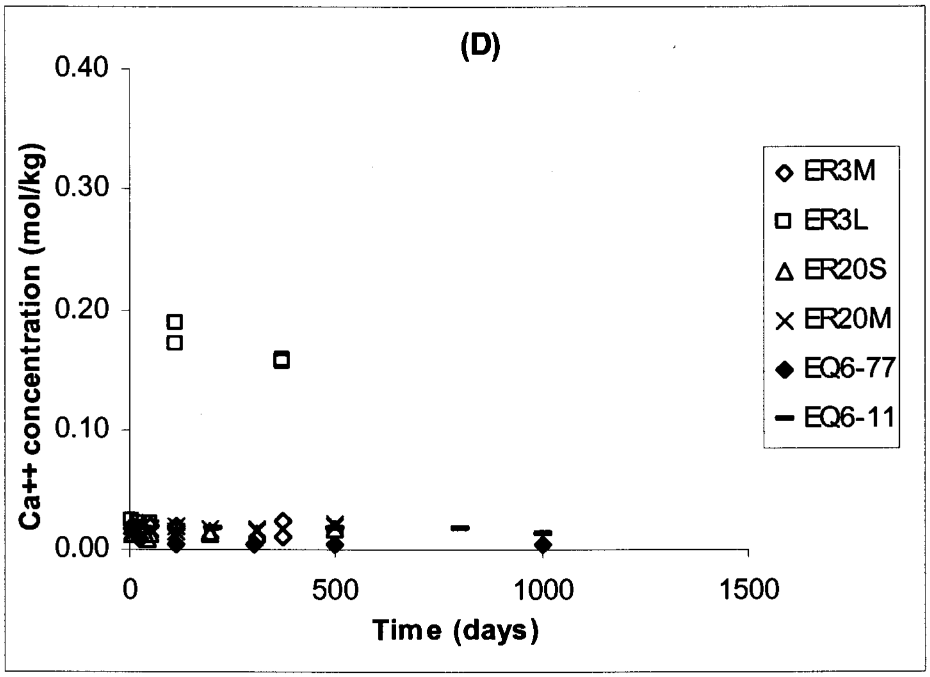


Figure 33. Plots showing experimental concentrations of (A) Mg^{2+}, (B) Cl^{-}, (C) pmH, and (D) Ca^{2++} versus time (days) for MM MgO hydrated in ERDA-6, and the results of the EQ3/6 modeling runs titrating periclase into simplified GWB brine. The experimental conditions corresponding to each ER series can be found in Table 1. The series EQ6-77 and EQ6-11 represent the EQ3/6 modeling runs of MgO hydrated in 77 ml and 11ml brine with arbitrary time scaling.

5 CONCLUSIONS

MgO hydration experiments were carried out with three MgO particle sizes and two solid-to-liquid ratios in three WIPP-related brines: ERDA-6, GWB and simplified GWB. The hydration products include brucite and phase-5. In addition to phase-5, MgO hydrated in simplified GWB or GWB produces brucite, while MgO hydrated in ERDA-6 only produces brucite. The MgO particle size seemed to have a significant effect on the formation of hydration products. Small MgO particles form hydration product before the large particles. MgO hydrated faster in simplified GWB compared to the other two brines.

An important, new finding in this study is the observation of formation of phase-5 in simplified GWB (ionic strength 7.9 m). This further supports the conclusion of Xiong and Lord (2008) that phase-5 is the stable phase in Mg-Na-Cl-dominated brine with an ionic strength up to 8.3 m similar to WIPP GWB. In contrast, phase-3 is the stable phase in the $MgCl_2$ saturated Q-brine with an ionic strength up to 15 m in the Asse repository.

We used EQ3/6 to simulate the reaction path way of MgO hydration and carbonation in a closed system containing brine and atmospheric carbon dioxide by titrating periclase into the system. Experimental values of pH, Mg^{+} concentration, Cl^{-} concentration, and hydration products were similar to the modeling predictions.

6 REFERENCES

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APPENDIX A

This appendix outlines the EQ3/6 calculations performed. Appendices A1-A6 describe the calculations. Appendix A7 gives the file names and file dependencies.

Appendix A1 EQ3/6 simulation of 3.0g MgO tritrated into 11 ml of ERDA-6

The purpose of the simulation is to titrate 3.0 g of MgO into a closed system containing 11 ml of ERDA-6 brine.
Step1. Make EQ3 input file for brine equilibrated with atmospheric concentration of carbon dioxide, using brine recipe of ERDA-6 from appendix B of SP20-4. Initial pH value and HCO^{2-} concentration were taken from Xiong et al. 2007 (section 3.1 and table 1).
Step2. Run EQ3.
Step3. Make EQ6 input file to titrate CaO into ERDA-6 brine. The amount of CaO is calculated in the Excel file "MgO in brine", worksheet "ERDA-6".
Step4. Run EQ6.
Step5. Make EQ6 input file to titrate MgO into ERDA-6 brine. The amount of MgO is calculated in the Excel file "MgO in brine", worksheet "ERDA-6".

Appendix A2 EQ3/6 simulation of 3.1g MgO titrated into 77 ml of ERDA-6
The purpose of the simulation is to titrate 3.1 g of MgO into a closed system containing 77 ml of ERDA-6 brine.
Step1. Make EQ3 input file for brine equilibrated with atmospheric concentration of carbon dioxide, using brine recipe of ERDA-6 from appendix B of SP20-4. Initial pH value and HCO^{2-} were taken from Xiong et al. 2007 (section 3.1 and table 1).
Step2. Run EQ3.
Step3. Make EQ6 input file to titrate CaO into ERDA-6 brine. The amount of CaO is calculated in the Excel file "MgO in brine", worksheet "ERDA-6".
Step4. Run EQ6.
Step5. Make EQ6 input file to titrate MgO into ERDA-6 brine. The amount of MgO is calculated in the Excel file "MgO in brine", worksheet "ERDA-6".

Appendix A3 EQ3/6 simulation of 3.0g MgO titrated into 11 ml of GWB

The purpose of the simulation is to titrate 3.0 g of MgO into a closed system containing 11 ml of GWB brine. Initial pH value and HCO^{2-} concentration were taken from Xiong et al. 2007 (section 3.1 and table 1), assuming HCO^{2-} concentration in GWB brine is the same as HCO^{2-} concentration in ERDA-6.
Step1. Make EQ3 input file for brine equilibrated with atmospheric concentration of carbon dioxide, using brine recipe of GWB from appendix B of SP20-4.
Step2. Run EQ3.
Step3. Make EQ6 input file to titrate MgO into GWB brine. The amount of MgO is calculated in the Excel file "MgO in brine", worksheet "GWB".
Step4. Run EQ6.

Appendix A4 EQ3/6 simulation of 3.1g MgO titrated into 77 ml of GWB

The purpose of the simulation is to titrate 3.1 g of MgO into a closed system containing 77 ml of GWB brine. Initial pH value and HCO^{2-} concentration were taken from Xiong et al 2007 (section 3.1 and table 1), assuming HCO^{2-} concentration in GWB brine is the same as HCO^{2-} concentration in ERDA-6.
Step1. Make EQ3 input file for brine equilibrated with atmospheric carbon dioxide, using brine recipe of GWB from appendix B of SP20-4.
Step2. Run EQ3
Step3. Make EQ6 input file to titrate MgO into GWB brine. The amount of MgO is calculated in the Excel file "MgO in brine", worksheet "GWB".
Step4. Run EQ6

Appendix A5 EQ3/6 simulation of 3.0g MgO titrated into 11 ml of simplified GWB

The purpose of the simulation is to titrate 3.0 g of MgO into a closed system containing 11ml of simplified GWB brine.
Step1. Make EQ3 input file for brine equilibrated with atmospheric concentration of carbon dioxide, using brine recipe for simplified GWB (1M MgCl2 + 3.6 M NaCl).
Step2. Run EQ3.
Step3. Make EQ6 input file to titrate MgO into GWB brine. The amount of MgO is calculated in the Excel file "MgO in brine", worksheet "SGWB".
Step4. Run EQ6.

Appendix A6 EQ3/6 simulation of 3.1g MgO titrated into 77 ml of simplified GWB

The purpose of the simulation is to titrate 3.1 g of MgO into a closed system containing 77 ml of GWB brine.
Step1. Make EQ3 input file for brine equilibrated with atmospheric concentration of carbon dioxide, using brine recipe for simplified GWB (1M MgCl2 + 3.6 M NaCl).
Step2. Run EQ3.
Step3. Make EQ6 input file to titrate MgO into GWB brine. The amount of MgO is calculated in the Excel file "MgO in brine", worksheet "SGWB".
Step4. Run EQ6.

Appendix A7 File naming convention for EQ3/6 runs

Table 1. File naming convention for the EQ3/6 runs

File Name	Description
erd.3i	EQ3 input file for ERDA-6 brine equilibrated with atmospheric concentration of carbon dioxide
erd.3p	EQ3 pickup file from erd.3i. This file will be used for EQ6 run simulating CaO titrated into ERDA-6
erd.3o	EQ3 output file from erd.3i
erdca-11.6i	EQ6 input file for CaO titrated into 11ml of ERDA-6 brine. This file is a descendent of erd.3p
erdca-11.6p	EQ6 pickup file from erdca-11.6i. This file will be used for EQ6 run simulating MgO titrated into ERDA-6
erdca-11.6o	EQ6 output from erdca-11.6i
erdca-12.6i	EQ6 input file for MgO titrated into 11ml of ERDA-6 brine, which has been reacted with CaO. This file is a descendent of erdca-11.6p
erdca-12.6p	EQ6 pickup file from erdca-12.6i
erdca-12.6o	EQ6 output file from erdca-12.6i
erdca-77.6i	EQ6 input file for CaO titrated into 77 ml of ERDA-6 brine. This file is a descendent of erd.3p
erdca-77.6p	EQ6 pickup file from erdca-77.6i. This file will be used for EQ6 run simulating MgO titrated into ERDA-6
erdca-77.6o	EQ6 output from erdca-77.6i
erdca-78.6i	EQ6 input file for MgO titrated into 77 ml of ERDA-6 brine, which was been reacted with CaO. This file is a descendent of erdca-77.6p
erdca-78.6p	EQ6 pickup file from erdca-78.6i
erdca-78.6o	EQ6 output file from erdca-78.6i
gwb.3i	EQ3 input file for GWB brine equilibrated with atmospheric concentration of carbon dioxide
gwb.3p	EQ3 pickup file from gwb.3i. This file will be used for EQ6 run simulating MgO titrated into GWB
gwb.3o	EQ3 output file from gwb.3i
gwb-11.6i	EQ6 input file for MgO titrated into 11ml of GWB brine. This file is a descendent of gwb.3p
gwb-11.6p	EQ6 pickup file from gwb-11.6i
gwb-11.6o	EQ6 output file from gwb-11.6i
gwb-77.6i	EQ6 input file for MgO titrated into 77ml of GWB brine. This file is a descendent of gwb.3p
gwb-77.6p	EQ6 pickup from gwb-77.6i
gwb-77.6o	EQ6 output file from gwb-77.6i
sgwbb.3i	EQ3 input file for simplified GWB brine equilibrated with atmospheric concentration of carbon dioxide
sgwbb.3p	EQ3 pickup file from sgwbb.3i. This file will be used for EQ6 run simulating MgO titrated into simplified GWB
sgwbb.3o	EQ3 output file from sgwbb.3i

sgwbb-11.6i	EQ6 input file for MgO titrated into 11ml of simplified GWB brine. This file is a descendent of sgwbb.3p
sgwbb-11.6p	EQ6 pickup file from sgwbb-11.6i
sgwbb-11.6o	EQ6 output file from sgwbb-11.6i
sgwbb-77.6i	EQ6 input file for MgO titrated into 77ml of simplified GWB brine. This file is a descendent of sgwbb.3p
sgwbb-77.6p	EQ6 pickup file from sgwbb-77.6i
sgwbb-77.6o	EQ6 output file from sgwbb-77.6i

Appendix B Microsoft Excel workbooks

File Name	Description
Brine acid base titration	Calculated pH conversion factor in section 3.3
Cl analysis	Calculated Cl concentration that was used in Excel file Plots~~(review)~~
ICPAES	Calculated Mg, Ca concentration used in Excel file Plots~~(review)~~
Plots	Generated figures in section 4.2-4.4
MgO in brine	Calculated the amount of MgO and CaO used in EQ3/6 input file

Trone, Janis R

From: Leigh, Christi D
Sent: Friday, May 15, 2009 1:28 PM
To: Trone, Janis R
Cc: Deng, Haoran
Subject: Re: Signature Authority

I authorize Janis Trone to sign the cover page for me for the report titled "Experimental Work Conducted on MgO Long-Term Hydration." I have signed the Management DRC already.

Christi Leigh
Manager 6712
Repository Investigations
Sandia National Laboratories
Carlsbad, NM
575-234-0038

APPENDIX A

This appendix outlines the EQ3/6 calculations performed supporting “Experimental work conducted on MgO long-term hydration”. The EQ3/6 files can be found in the CD. There will not be printed copy for this data package.

Appendix B Microsoft Excel workbooks

This appendix includes data files used in the MgO report, “Experimental work conducted on MgO long-term hydration”. Total of 63 pagea of data sheets is attached to Appendix B.

File Name	Description
Brine acid base titration	Calculated pH conversion factor in section 3.3
Cl analysis	Calculated Cl concentration that used in Excel file Plots
ICPAES	Calculated Mg, Ca concentration used in Excel file Plots
Plots	Generated figures in section 4.2-4.4
MgO in brine	Calculated the amount of MgO and CaO used in EQ3/6 input file

2/6/2007	Collection Date	Time (days	XRD	B/P(18/43)	Brucite mol%	pH	Cl- IC (mole/l)	True Mg mole/l	True Ca mole/l
ER20-S1	2/13/2007	7		0	5.54	8.67	0.00	2.29E-02	1.66E-02
ER20-S2	2/13/2007	7			5.06	8.56	0.00	2.15E-02	1.13E-02
ER20-S3	3/2/2007	24	P,H		14.67	8.98	0.00	0.00E+00	0.00E+00
ER20-S4	3/2/2007	24			28.4	8.96	0.00	0.00E+00	0.00E+00
ER20-S5	3/19/2007	41	P,B,H	0.085714	33.68	9.35	0.00	1.46E-02	8.33E-03
ER20-S6	3/19/2007	41			33.73	9.28	0.00	1.37E-02	7.86E-03
ER20-S7	3/28/2007	50	P,B,H,12	0.166667		9.39	4.54	1.76E-02	1.12E-02
ER20-S8	3/28/2007	50	P,B,H,12			9.40	4.34	1.60E-02	1.12E-02
ER20-S9	4/16/2007	69	P,B,12	0.189655		9.42	0.00		
ER20-S10	4/16/2007	69				9.36	0.00		
ER20-S11	5/30/2007	113	P,B,H,12	0.35		9.37	4.51		
ER20-S12	5/30/2007	113				9.34	4.48		
ER20S13	8/23/2007	198	P,B,H,12	0.441176		9.40	4.54	9.89E-02	1.18E-02
ER20S14	8/23/2007	198				9.49	4.12	8.42E-02	1.28E-02
ER20S15	12/11/2007	308	P,B,H,12	0.6		9.45	4.67	0.00E+00	1.22E-02
ER20S16	12/11/2007	308				9.42	4.71	0.00E+00	1.21E-02
ER20S17	6/18/2008	498	P,B,H,12	0.15625		9.33	4.41	1.17E-02	1.45E-02
ER20S18	6/18/2008	498				9.40	4.37	1.28E-02	1.52E-02
ER3-M	Collection Date		XRD	B/P(18/43)	Brucite mol%	pH	Cl- IC (mole/l)	True Mg mole/l	True Ca mole/l
ER3-M1	2/13/2007	7				9.16	0.00	1.47E-02	1.60E-02
ER3-M2	2/13/2007	7	P,H			9.13	0.00	1.39E-02	1.65E-02
ER3-M3	3/2/2007	24	P,H		3.06	9.76	2.21	7.56E-03	1.53E-02
ER3-M4	3/2/2007	24				9.74	4.81	5.97E-03	1.53E-02
ER3-M5	3/28/2007	50	P,B,H	0.04	8.47	10.40	5.04		1.70E-02
ER3-M6	3/28/2007	50	P,B,H		2.92	10.40	5.00		1.76E-02
ER3-M7	5/30/2007	113	P,B,H,12	0.06		11.06	4.46		1.63E-02
ER3-M8	5/30/2007	113				11.11	4.40		1.64E-02
ER3-M9	2/12/2008	371	P,B H	0.153846		10.88	4.52	0.00E+00	2.10E-02
ER3-M10	2/12/2008	371				9.41	5.06	0.00E+00	9.08E-03

1 Collection Date in column B can be found in notebook WIPP-MMMgO-5, p60-71
2 Time in column C = collection date in column B - starting date in cell A1 (the starting date can be found in WIPP-MMMgO-5, p60-71)
3 Column XRD, B/P(18/43) and Brucite mol% are not usded in the report
4 pH in column G can be found in notebook WIPP-MMMgO-5, p60-71.
5 Cl -IC (mole/l) in column H can be found in Excell file "Cl analysis", column D.
6 True Mg mol/l in column I can be found in excell file "ICP-AES" column G.
7 True Ca mol/l in column J can be found in excell file "ICP-AES" column H.

ER20-M	Collection Date	Time (day)	XRD	B/P(18/43)	Brucite mol%	pH	Cl IC (mole/l)	True Mg mole/l	True Ca mole/l
ER20-M1	2/13/2007	7			0.55	8.42		2.07E-02	1.31E-02
ER20-M2	2/13/2007	7			0.5	8.48		2.05E-02	1.25E-02
ER20-M3	3/2/2007	24	P,H		1.01	8.80	4.38	0.00E+00	0.00E+00
ER20-M4	3/2/2007	24				9.17	4.36	0.00E+00	0.00E+00
ER20-M5	3/28/2007	50	P,H		7.67	9.54	4.83	1.01E-02	1.60E-02
ER20-M6	3/28/2007	50	P,H		7.3	9.42	4.72	1.73E-02	1.63E-02
ER20-M7	5/30/2007	113	P,H,B,12	0.0606061		9.39	4.68	6.97E-03	1.41E-02
ER20-M8	5/30/2007	113				9.41	4.58	8.31E-03	1.67E-02
ER20-M9	8/23/2007	198	P,H,B,12	0.0769231		9.61	5.08	1.60E-02	1.49E-02
ER20-M10	8/23/2007	198				9.63	4.33	1.25E-02	1.51E-02
ER20-M11	12/11/2007	308	P,H,B,12	0.171875		9.53	4.69	0.00E+00	1.56E-02
ER20-M12	12/11/2007	308				9.52	4.67	0.00E+00	1.40E-02
ER20-M13	6/18/2008	498		0.2058824		9.47	0.00	6.62E-03	1.88E-02
ER20-M14	6/18/2008	498	P,H,B,12			9.48	4.37	6.81E-03	1.80E-02

ER3-L	Collection Date		XRD	B/P(18/43)	Brucite mol%	pH	Cl IC (mole/l)	True Mg mole/l	True Ca mole/l
ER3-L1	2/13/2007	7			0.86	9.16	0.00	8.00E-02	2.15E-02
ER3-L2	2/13/2007	7	P,H		0.83	9.13	0.00	1.97E-02	2.08E-02
ER3-L3	3/2/2007	24	P		1.64	9.76	4.64	2.89E-03	1.97E-02
ER3-L4	3/2/2007	24				9.74	4.72	2.81E-03	1.95E-02
ER3-L5	3/28/2007	50	P,H		1.73	10.40	5.04		1.85E-02
ER3-L6	3/28/2007	50			2.02	10.40	4.95		1.94E-02
ER3-L7	5/30/2007	113	B,P	0.0697674		10.98	5.00		1.68E-01
ER3-L8	5/30/2007	113				10.98	5.52		1.53E-01
ER3-L9	2/12/2008	371	P,B,H	0.15625		9.97	5.03	1.90E-01	1.41E-01
ER3-L10	2/12/2008	371				9.79	4.82	1.85E-01	1.40E-01
									0.00E+00
									0.00E+00

GW20-M	Collection Date	Time (day)	XRD	M/P(12/43)	B/P(18/43	XRD	Brucite mol%	pH	Cl- IC (mole/l)	True Mg mole/l	True Ca mole/l
GW20-M1	2/13/2007	7					0.6	7.46	0.00	0.00E+00	1.18E-02
GW20-M2	2/13/2007	7					0.54	7.44	0.00	0.00E+00	1.32E-02
GW20-M3	3/2/2007	24	P				2.62	7.94	4.93	8.57E-01	1.11E-02
GW20-M4	3/2/2007	24						7.92	5.03	8.16E-01	1.06E-02
GW20-M5	3/28/2007	50					5.45	8.11	5.34	0.00E+00	1.37E-02
GW20-M6	3/28/2007	50					3.39	8.09	5.01	0.00E+00	1.37E-02
GW20-M7	5/30/2007	113	P					8.24	4.99	0.00E+00	1.53E-02
GW20-M8	5/30/2007	113						8.26	5.07	0.00E+00	1.41E-02
GW20-M9	8/23/2007	198	P					8.38	5.11	1.12E+00	1.68E-02
GW20-M10	8/23/2007	198						8.39	5.01	1.13E+00	1.73E-02
GW20-M11(flack)	2/12/2008	371	P,H,M	0.2				8.34	5.28	1.07E+00	2.50E-02
GW20-M12	2/12/2008	371						8.35	5.03	1.03E+00	2.39E-02

GW20-M	Collection Date		XRD	M/P(12/43)	B/P(18/43	XRD	Brucite mol%	pH	Cl- IC (mole/l)	True Mg mole/l	True Ca mole/l
GW3-S1	2/13/2007	7					8.81	7.85			1.97E-02
GW3-S2	2/13/2007	7					8.44	8			
GW3-S3	3/2/2007	24						8.4	3.32	7.24E-01	1.76E-02
GW3-S4	3/2/2007	24	P,M,H	0.0857143	0		24.76	8.34	3.33	6.72E-01	1.68E-02
GW3-S5	3/19/2007	41	P,M	0.1060606	0			8.39		6.45E-01	1.43E-02
GW3-S6	3/19/2007	41					35.28	8.38		5.73E-01	1.52E-02
GW3-S7	3/28/2007	50	P,M,H,B	0.109375	0		38.42	8.34	5.47		1.58E-02
GW3-S8	3/28/2007	50	P,M,H	0.1206897	0		36.71	8.34	5.17		1.67E-02
GW3-S9(wet grou	4/16/2007	69	P,M	0.0882353	0			8.38			1.66E-02
GW3-S10	4/16/2007	69						8.37		7.18E-01	1.76E-02
[redacted]	**5/30/2007**	113	**P,B,M,H**	0.1851852	0.0740741			8.35	5.26	7.25E-01	1.83E-02
GW3-S12	5/30/2007	113	P,B,M					8.36	5.15	7.05E-01	1.73E-02
GW3-S13	**8/23/2007**	198	**P,B,M,H**	0.2972973	0			8.39	4.85	8.85E-01	1.74E-02
GW3-S14	8/23/2007	198						8.4	5.08	8.85E-01	1.71E-02
GW3-S15	**12/11/2007**	308	**P,B,M,H**	0.1875	0.0625			8.39	5.46	8.42E-01	1.49E-02
GW3-S16	12/11/2007	308						8.36	5.24	8.75E-01	1.51E-02
GW3-S17	6/18/2008	498		0.0909091	0.0454545			8.3	6.13	7.90E-01	2.22E-02
GW3-S18	6/18/2008	498						8.39	5.03	6.53E-01	1.87E-02

GW20-L	Collection Date	Time (day)	XRD	M/P(12/43	B/P(18/43	XRD (Rewash	Brucite mol%	pH	Cl- IC (mole/l)	True Mg mole/l	True Ca mole/l
GW20-L1	2/13/2007	7					1.05	7.3	0.00	0.00E+00	1.29E-02
GW20-L2	2/13/2007	7	P,H				1.33	7.33	0.00	0.00E+00	1.32E-02
GW20-L3	3/2/2007	24	P,H				1.94	7.54	5.22	0.00E+00	0.00E+00
GW20-L4	3/2/2007	24						7.6	9.43	0.00E+00	0.00E+00
GW20-L5	3/28/2007	50	P,H			P	0.83	7.79	5.67	0.00E+00	1.39E-02
GW20-L6	3/28/2007	50	P,H			P	2.14	7.78	5.66	0.00E+00	1.38E-02
GW20-L7	5/30/2007	113	P,H			P		8.07	5.11	0.00E+00	1.58E-02
GW20-L8	5/30/2007	113	P,H					8.06	5.11	0.00E+00	1.71E-02
GW20-L9	8/23/2007	198	P,H					8.32	4.69	1.20E+00	1.63E-02
GW20-L10	8/23/2007	198						8.31	5.07	1.20E+00	1.68E-02
GW20-L11	2/12/2008	371	P, H					8.34	4.62	1.03E+00	2.39E-02
GW20-L12	2/12/2008	371						8.35	4.99	1.13E+00	2.47E-02

GW3-M	Collection Date		XRD	M/P(12/43	B/P(18/43	XRD (Rewash	Brucite mol%	pH	Cl- IC (mole/l)	True Mg mole/l	True Ca mole/l
GW3-M1	2/13/2007	7					0.85	7.85	0.00	9.05E-01	1.43E-02
GW3-M2	2/13/2007	7	P				0.98	8	0.00	8.86E-01	1.48E-02
GW3-M3	3/2/2007	24	P,H				6.48	8.4	5.16	7.89E-01	1.53E-01
GW3-M4	3/2/2007	24						8.34	5.34	[redacted]	1.85E-01
GW3-M5	3/28/2007	50	P,M,B,H	0.057692			5.85	8.39	4.87	8.38E-01	1.52E-02
GW3-M6	3/28/2007	50	P				8.04	8.38	5.46	7.82E-01	1.40E-02
GW3-M7	5/30/2007	113	P,M,B,H	0.222222	0	P,M,B		8.39	4.86	7.61E-01	1.81E-02
GW3-M8	5/30/2007	113						8.37	4.90	6.95E-01	1.62E-02
GW3-M9	**8/23/2007**	198	**P**	0				8.47	4.85	7.76E-01	1.70E-02
GW3-M10	8/23/2007	198						8.43	0.00	7.76E-01	1.72E-02
GW3-M11	12/11/2007	308	P,M,B,H	0.246154	0.061538			8.36	5.33	7.67E-01	1.52E-02
GW3-M12	12/11/2007	308						8.37	5.26	7.57E-01	1.56E-02
GW3-M13	6/18/2008	498		0.192308	0.115385			8.31	4.44	5.91E-01	1.86E-02
GW3-M14	6/18/2008	498						8.35	5.92	6.81E-01	2.16E-02

MgCL20-M	Collection Date	Time (day)	XRD	M/P(12/43)	B/P(18/43	XRD (Rewash	Brucite mol%	pH	Cl IC (mole/l)	True Mg mole/l	True Ca mole/l
MgCL20-M1	2/13/2007	7					10.26	8.18	0.00	0.00E+00	4.91E-03
MgCL20-M2	2/13/2007	7					11.54	8.18	0.00	0.00E+00	4.54E-03
MgCL20-M3	3/2/2007	24	P,M,B,H	0.230769231	0		46.48	8.16	0.00	8.25E-01	4.75E-03
MgCL20-M4	3/2/2007	24						8.18	0.00	8.55E-01	4.84E-03
MgCL20-M5	3/19/2007	41	P,M,B,H	0.615384615	0.269230769			8.12	0.00	6.64E-01	4.84E-03
MgCL20-M6	3/19/2007	41					92.6	8.13	0.00	0.00E+00	4.87E-03
MgCL20-M7	3/28/2007	50	P,M,B,H	0.9	0.45		106.68	8.1	5.54	0.00E+00	5.34E-03
MgCL20-M8	3/28/2007	50					104.66	8.09	6.07	0.00E+00	5.56E-03
MgCL20-M9(soak over night)	4/16/2007	69	P,B,M,H	0.428571429	1.857142857			8.11	0.00	0.00E+00	5.26E-03
MgCL20-M10	4/16/2007	69						8.09	0.00	0.00E+00	5.88E-03
MgCL20-M11	5/30/2007	113	P,B,M,H	2.34375	1.71875	P,B,M,H		8.09	5.39	0.00E+00	5.24E-03
MgCL20-M12	5/30/2007	113						8.13	5.55	0.00E+00	5.05E-03
MgCL20-M13	7/16/2007	160	P,B,M,H	2.96875	2.5			8.13	5.99	9.04E-01	1.67E-02
MgCL20-M14	7/16/2007	160	P,B,M,H					8.14	6.14	7.76E-01	1.69E-02
MgCl20M-15	8/23/2007	198						8.17	4.57	9.56E-01	5.48E-03
MgCl20M-16	8/23/2007	198	P,B,M	3.666666667	3.333333333			8.18	4.86	1.03E+00	5.65E-03
MgCl20M-17	12/11/2007	308	P,B,M,H	5.714285714	3.857142857			8.19	5.91	1.10E+00	6.50E-03
MgCl20M-18	12/11/2007	308						8.22	5.70	1.09E+00	5.04E-02
MgCl20M19	4/17/2008	436	P,B,M,H	8.25	7.875			8.17	5.32	1.09E+00	6.32E-03
MgCl20M20	4/17/2008	436						8.16	5.20	1.08E+00	6.15E-03

MgCL3-S	Collection Date		XRD	M/P(12/43)	B/P(18/43	XRD (Rewash	Brucite mol%	pH	Cl IC (mole/l)	True Mg mole/l	True Ca mole/l
MgCL3-S1	2/13/2007	7					33.52	8.32	0.00	0.00E+00	3.07E-02
MgCL3-S2	2/13/2007	7					32.88	8.31	0.00	0.00E+00	3.16E-02
MgCL3-S3	3/2/2007	24	P,M,B,H	0.294117647	0.176470588	P,B		8.34	5.65	0.00E+00	3.43E-02
MgCL3-S4	3/2/2007	24						8.35	0.00	5.95E-01	3.50E-02
MgCL3-S5	3/19/2007	41	P,M,B,H	0.433333333	0.333333333			8.24	5.74	4.57E-01	3.60E-02
MgCL3-S6	3/19/2007	41						8.24	0.00	3.61E-01	3.60E-02
MgCL3-S7	3/28/2007	50	P,M,B,H	0.5	0.464285714			8.25	5.32	0.00E+00	3.94E-02
MgCL3-S8	3/28/2007	50						8.25	5.17	0.00E+00	4.05E-02
MgCL3-S9 (wet ground)	4/16/2007	69	P,M, B	0.3125	0.53125			8.23	0.00	0.00E+00	4.33E-02
MgCL3-S10	4/16/2007	69					90.1	8.23	0.00	0.00E+00	5.01E-02
MgCL3-S11	5/30/2007	113	P,B,M,H	0.636363636	0.909090909			8.21	5.20	0.00E+00	4.55E-02
MgCl3-S12	5/30/2007	113						8.21	5.18	0.00E+00	4.70E-02
MgCL3-S13	7/16/2007	160						8.32	5.65	5.68E-01	6.63E-02
MgCL3-S14	7/16/2007	160	P,B,M,H	1	1.272727273			8.26	5.81	5.87E-01	6.40E-02
MgCl3-S15	8/23/2007	198	P,B,M,H	1.6	2.4			8.28	5.51	7.57E-01	5.39E-02
MgCl3-S16	8/23/2007	198						8.28	5.22	7.52E-01	5.31E-02
MgCl3-S17	12/11/2007	308	P,M,B,H	2.928571429	3.928571429			7.99	5.54	7.48E-01	5.02E-02
MgCl3-S18	12/11/2007	308						8.01	5.64	7.85E-01	5.70E-03
MgCl3-S19	4/17/2008	436	P,M,B,H	2.625	7.625			8.16	5.36	8.56E-01	5.13E-02
MgCl3-S20	4/17/2008	436						8.19	5.40	8.09E-01	4.73E-02
MgCl3-S21	6/18/2008	498						8.14	5.48	7.10E-01	5.97E-02
MgCl3-S22	6/18/2008	498						8.15	5.19	7.05E-01	5.74E-02

MgCL20-L	Collection Date	Time (	XRD	M/P(12/	B/P(1	XRD (Rewash)				Brucite mol%	pH	Cl IC (mole/l)	True Mg mole/l	True Ca mole/l
MgCL20-L1	2/13/2007	7								4.2	8.21	0.00	0.00E+00	4.50E-03
MgCL20-L2	2/13/2007	7								4.24	8.25	0.00	0.00E+00	6.57E-03
MgCL20-L3	3/2/2007	24	P,M,H	0.16	0.02	P					8.11	0.00	8.71E-01	4.67E-03
MgCL20-L4	3/2/2007	24									8.17	0.00	8.74E-01	4.47E-03
MgCL20-L5	3/19/2007	41	P,B,M.H	0.4444	0.33	Blur n	70C,3hr				8.12	0.00	7.68E-01	4.55E-03
MgCL20-L6	3/19/2007	41	P,H								8.09	0.00	6.78E-01	4.59E-03
MgCL20-L7	3/28/2007	50	P,B,M.H	0.6429	0.57	methanol				76.59	8.12	5.47	0.00E+00	5.50E-03
MgCL20-L8	3/28/2007	50	P,B,M.H	0.64	0.68	P,B,M				76.64	8.14	5.19	0.00E+00	4.96E-03
MgCL20-L9(wet gr	4/16/2007	69	P,B,M	1	1.7						8.11	0.00	0.00E+00	5.16E-03
MgCL20-L10	4/16/2007	69									8.08	0.00	0.00E+00	5.25E-03
MgCL20-L11	5/30/2007	113	P,M,B,H	0.8462	1.77						8.09	5.62	0.00E+00	5.38E-03
MgCL20-L12	5/30/2007	113									8.11	5.28	0.00E+00	5.30E-03
MgCL20-L13	7/16/2007	160	P,B,M,H	2.75	3.25						8.12	5.94	9.32E-01	1.69E-02
MgCL20-L14	7/16/2007	160	P,B,M,H								8.07	5.94	8.85E-01	1.71E-02
MgCL20-L15	8/23/2007	198	P,B,M,H	3.1667	3.67						8.15	5.27	1.24E+00	5.97E-03
MgCL20-L16	8/23/2007	198									8.14	5.31	1.16E+00	6.34E-03
MgCL20-L17	12/11/2007	308	P,B,M,H	7.2	6.8						7.99	5.58	1.12E+00	5.97E-03
MgCL20-L18	12/11/2007	308									8.01	5.65	1.12E+00	5.28E-03
MgCL20-L19	4/17/2008	436	P,M,B,H	6.25	7.13						8.15	5.35	1.15E+00	6.21E-03
MgCL20-L20	4/17/2008	436									8.16	5.51	1.14E+00	5.82E-03

MgCL3-M	Collection Date		XRD	M/P(12/	B/P(1	XRD (Rewash		M/P(1	B/P(1	Brucite mol%	pH	Cl IC (mole/l)	True Mg mole/l	True Ca mole/l
MgCL3-M1	2/13/2007	7								3.14	8.25	0.00	0.00E+00	3.18E-02
MgCL3-M2	2/13/2007	7								4.09	8.24	0.00	0.00E+00	3.18E-02
MgCL3-M3	3/2/2007	24	P,M,H	0.1429	0	P	3hr, 70	0.088	0	37.09	8.28	5.57	7.13E-01	3.21E-02
MgCL3-M4	3/2/2007	24									8.29	0.00	7.43E-01	3.18E-02
MgCL3-M5	3/19/2007	41	P,B,M,H	0.2564	0.31						8.18	0.00	5.24E-01	3.49E-02
MgCL3-M6	3/19/2007	41								60.8	8.17	0.00	5.01E-01	3.38E-02
MgCL3-M7	3/28/2007	50				P,B,M,	methno	0.313	0.57	71.16	8.2	5.21	0.00E+00	4.09E-02
MgCL3-M8	3/28/2007	50	P,B,M,H	0.4545	0.48		70C, ov	0.15+(	0.53	74.49	8.17	5.16	0.00E+00	4.21E-02
MgCL3-M9	4/16/2007	69	P,B,M,H	1	1.7	P,B,M,	wet gro	1	1.7		8.16	0.00	6.95E-01	4.75E-02
MgCL3-M10	4/16/2007	69									8.16	0.00	6.34E-01	4.27E-02
MgCL3-M11	5/30/2007	113	P,B,M,H	0.4706	1.29						8.16	5.25	6.54E-01	4.75E-02
MgCL3-M12	5/30/2007	113									8.16	5.45	6.87E-01	5.04E-02
MgCL3-M13	7/16/2007	160									8.26	9.78	6.72E-01	6.03E-02
MgCL3-M14	7/16/2007	160	P,B,M,H	1.0667	1.6						8.21	5.87	6.62E-01	6.40E-02
MgCL3-M15	8/23/2007	198	P,B,M,H	1.7273	2.18						8.26	5.47	8.47E-01	5.02E-02
MgCL3-M16	8/23/2007	198									8.26	5.34	8.61E-01	5.34E-02
MgCL3-M17	12/11/2007	308									8.19	5.47	8.47E-01	4.92E-02
MgCL3-M18	12/11/2007	308	P,B,M,H	2.95	4.2						8.22	5.43	8.23E-01	4.82E-02
MgCl3-M19	4/17/2008	436	P,M,B,H	1.3	4.35						8.16	5.39	9.13E-01	5.05E-02
MgCl3-M20	4/17/2008	436	P,M,B,H	1	4.13						8.19	5.40	8.52E-01	5.01E-02
MgCl3-M21	6/18/2008	498	P,M,B,H	2.7273	7.5						8.15	5.53	6.86E-01	6.26E-02
MgCl3-M22	6/18/2008	498									8.18	5.58	6.43E-01	5.91E-02

1				Log (molarity to molality) 0.049857161	molarity to molality 1.121649485	H+ log gamma 0.7569	A (pH correction factor) 1.155		Cl- log gamma -0.2666		Mg++ log gamma 0.5634		aw 0.788847		Brucite log k 17.1090	Phase 5 log k 43.1900	Phase 3 log k 26.0297
2/6/2007	Collection Date	Time (days)	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl- concentration (mol/l)	Cl- concentration (mol/kg)	Mg++ concentration (mol/l)	Mg++ concentration (mol/kg)	Ca++ concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase5)	SI (phase 3)
ER20-S1	2/13/2007	7	NA	NA	NA	8.67	9.83	9.78	NA		2.29E-02	2.57E-02	1.66E-02	1.87E-02	-0.31		
ER20-S2	2/13/2007	7	NA	NA	NA	8.56	9.72	9.67	NA		2.15E-02	2.42E-02	1.13E-02	1.27E-02	-0.55		
ER20-S3	3/2/2007	24	NA	NA	NA	8.98	10.14	10.09	NA		NA		NA				
ER20-S4	3/2/2007	24	NA	NA	NA	8.96	10.12	10.07	NA		NA		NA				
ER20-S5	3/19/2007	41	NA	NA	NA	9.35	10.51	10.46	NA		1.46E-02	1.64E-02	8.33E-03	9.34E-03	0.86		
ER20-S6	3/19/2007	41	NA	NA	NA	9.28	10.44	10.39	NA		1.37E-02	1.53E-02	7.86E-03	8.82E-03	0.69		
ER20-S7	3/28/2007	50	NA	NA	NA	9.39	10.55	10.50	4.54	5.10	1.76E-02	1.97E-02	1.12E-02	1.26E-02	1.02	1.59	0.62
ER20-S8	3/28/2007	50	NA	NA	NA	9.40	10.56	10.51	4.34	4.87	1.60E-02	1.80E-02	1.12E-02	1.26E-02	1.00	1.50	0.55
ER20-S9	4/16/2007	69	NA	NA	NA	9.42	10.58	10.53	NA		NA		NA				
ER20-S10	4/16/2007	69	NA	NA	NA	9.36	10.52	10.47	NA		NA		NA				
ER20-S11	5/30/2007	113	NA	NA	NA	9.37	10.53	10.48	4.51	5.06	NA		NA				
ER20-S12	5/30/2007	113	NA	NA	NA	9.34	10.50	10.45	4.48	5.03	NA		NA				
ER20S13	8/23/2007	198	NA	NA	NA	9.40	10.56	10.51	4.54	5.09	9.89E-02	1.11E-01	1.18E-02	1.32E-02	1.79	3.89	2.15
ER20S14	8/23/2007	198	NA	NA	NA	9.49	10.65	10.60	4.12	4.63	8.42E-02	9.45E-02	1.28E-02	1.44E-02	1.90	4.09	2.24
ER20S15	12/11/2007	308	NA	NA	NA	9.45	10.61	10.56	4.67	5.24	NA		1.22E-02	1.37E-02			
ER20S16	12/11/2007	308	NA	NA	NA	9.42	10.58	10.53	4.71	5.29	NA		1.21E-02	1.36E-02			
ER20S17	6/18/2008	498	NA	NA	NA	9.33	10.49	10.44	4.41	4.95	1.17E-02	1.31E-02	1.45E-02	1.63E-02	0.72	0.74	0.07
ER20S18	6/18/2008	498	NA	NA	NA	9.40	10.56	10.51	4.37	4.90	1.28E-02	1.44E-02	1.52E-02	1.70E-02	0.90	1.21	0.36

						H+ log gamma 0.7524			Cl- log gamma -0.2664		Mg++ log gamma 0.5502		aw 0.788766				
ER3-M	Collection Date	Time (days)	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase5)	SI (phase 3)
ER3-M1	2/13/2007	7	NA	NA	NA	9.16	10.32	10.27	0.00	0.00	1.47E-02	1.65E-02	1.60E-02	1.79E-02	0.48		
ER3-M2	2/13/2007	7	NA	NA	NA	9.13	10.29	10.24	0.00	0.00	1.39E-02	1.55E-02	1.65E-02	1.85E-02	0.39		
ER3-M3	3/2/2007	24	NA	NA	NA	9.76	10.92	10.87	2.21	2.47	7.56E-03	8.48E-03	1.53E-02	1.72E-02	1.39	2.01	0.67
ER3-M4	3/2/2007	24	NA	NA	NA	9.74	10.90	10.85	4.81	5.39	5.97E-03	6.69E-03	1.53E-02	1.72E-02	1.25	1.94	0.69
ER3-M5	3/28/2007	50	NA	NA	NA	10.40	11.56	11.51	5.04	5.65	NA		1.70E-02	1.90E-02			
ER3-M6	3/28/2007	50	NA	NA	NA	10.40	11.56	11.51	5.00	5.60	NA		1.76E-02	1.98E-02			
ER3-M7	5/30/2007	113	NA	NA	NA	11.06	12.22	12.17	4.46	5.00	NA		1.63E-02	1.83E-02			
ER3-M8	5/30/2007	113	NA	NA	NA	11.11	12.27	12.22	4.40	4.93	NA		1.64E-02	1.84E-02			
ER3-M9	2/12/2008	371	NA	NA	NA	10.88	12.04	11.99	4.52	5.07	NA		2.10E-02	2.36E-02			
ER3-M10	2/12/2008	371	NA	NA	NA	9.41	10.57	10.52	5.06	5.67	NA		9.08E-03	1.02E-02			

Constants:	
	Molarity to molality conversion factor for ERDA-6 in cell F5 = Concentration of Na+ (mol/L) /Concentration of Na+ (mol/kg) = 5.44/4.85
	The molar and molal Na+ concentrations are given in SP20-4 Appendix B
	For the H+ log gamma in cell G5 and cell G29 see the explanation section of worksheet "Fig 33" of this Excel file.
	The pH correction factor A in cell H5 can be found in Excel file " Brine acid base titration", worksheet "sum"
	For the Cl- log gamma in J5/29 see the explanation section of worksheet "Fig 33" of this Excel file.
	For the Mg++ log gamma in cells L5/29 see the explanation section of worksheet "Fig 33" of this Excel file.
	For the activity of water (aw) in N5/29 see the explanation section of worksheet "Fig 33" of this Excel file.
	Log k for brucite in cell P5 = 17.1090
	Log k for phase-5 in cell Q5 = 43.19
	L:og k for phase-3 in cell R5 = 26.0297
	These Log K's can be found in the EQ3/6 database: data0.hmo, and in the memo: Xiong et al., 2009
Calculations:	Time in column C = collection date in column B - starting date in cell A6 (data in column B and cell A6 can be found in WIPP-MMMgO-5, p60-71)
	Column D, E, F are not used
	pH in column G can be found in notebook WIPP-MMMgO-5, p60-71.
	pcH in column H = pH in column G + A (pH correction factor) in Cell H5
	pmH in column I = pcH in column H + log (molarity to molality conversion factor in Cell F5)
	Cl concentration (mole/l) in column J can be found in Excel file "Cl analysis", column D.
	Cl concentration (mol/kg) in column K = Cl concentration (mol/l) in column J x molar conversion factor in cell F5
	Mg concentration (mol/l) in column L can be found in excel file "ICP-AES" column G.
	Mg concentration (mol/kg) in column M = Mg concentration (mol/l) in column L x molar conversion factor in cell F5
	Ca concentration (mol/l) in column N can be found in excel file "ICP-AES" column H.
	Ca concentration (mol/kg) in column O = Ca concentration (mol/l) in column N x molar conversion factor in cell F5
	SI of brucite in column P, see subsection 4.2 of the report
	"=log (Mg concentration in column M) + Mg log gamma in cell L5/29 + 2 pmH in column I- 2 H log gamma in cell G5/29
	+ 2 log aw in cell N5 - log k of brucite in cell P5
	SI of phase-5 in column Q, see subsection 4.2 of report
	"=3 log (Mg concentration mol/kg in column M)+ 3 Mg log gamma in cell L5/29 + 5 pmH in column I
	"- 5 H log gamma in cell G5/29+ 9 log Aw in cell N5/29"
	"+ log (Cl concentration in column K) + Cl log gamma in cell J5/29 - log k of phase-5 in cell Q5"
	SI of phase-3 in column Q , see subsection 4.2 of report
	"=2 log (Mg concentration in column M)+ 2 Mg log gamma in cell L5/29 + 3 pmH in column I
	"- 3 H log gamma in cell G5/29+ 7 log aw in cell N5/29"
	"+ log (Cl concentration in column K) + Cl log gamma in cell J5/29 -log k of phase-3 in cell R5"

ER20-M	Collection Date	Time (days)	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase5)	SI (phase 3)
ER20-M1	2/13/2007	7	NA	NA	NA	8.42	9.58	9.53	NA		2.07E-02	2.33E-02	1.31E-02	1.46E-02	-0.85		
ER20-M2	2/13/2007	7	NA	NA	NA	8.48	9.64	9.59	NA		2.05E-02	2.30E-02	1.25E-02	1.40E-02	-0.73		
ER20-M3	3/2/2007	24	NA	NA	NA	8.80	9.96	9.91	4.38	4.91	NA		NA				
ER20-M4	3/2/2007	24	NA	NA	NA	9.17	10.33	10.28	4.36	4.88	NA		NA				
ER20-M5	3/28/2007	50	NA	NA	NA	9.54	10.70	10.65	4.83	5.42	1.01E-02	1.13E-02	1.60E-02	1.80E-02	1.08	1.64	0.56
ER20-M6	3/28/2007	50	NA	NA	NA	9.42	10.58	10.53	4.72	5.30	1.73E-02	1.94E-02	1.63E-02	1.82E-02	1.07	1.73	0.66
ER20-M7	5/30/2007	113	NA	NA	NA	9.39	10.55	10.50	4.68	5.24	6.97E-03	7.82E-03	1.41E-02	1.58E-02	0.62	0.40	-0.22
ER20-M8	5/30/2007	113	NA	NA	NA	9.41	10.57	10.52	4.58	5.14	8.31E-03	9.32E-03	1.67E-02	1.87E-02	0.73	0.72	-0.02
ER20-M9	8/23/2007	198	NA	NA	NA	9.61	10.77	10.72	5.08	5.70	1.60E-02	1.80E-02	1.49E-02	1.68E-02	1.42	2.62	1.20
ER20-M10	8/23/2007	198	NA	NA	NA	9.63	10.79	10.74	4.33	4.85	1.25E-02	1.41E-02	1.51E-02	1.70E-02	1.35	2.33	0.98
ER20-M11	12/11/2007	308	NA	NA	NA	9.53	10.69	10.64	4.69	5.26	NA		1.56E-02	1.75E-02			
ER20-M12	12/11/2007	308	NA	NA	NA	9.52	10.68	10.63	4.67	5.24	NA		1.40E-02	1.57E-02			
ER20-M13	6/18/2008	498	NA	NA	NA	9.47	10.63	10.58	NA		6.62E-03	7.43E-03	1.88E-02	2.10E-02	0.76		
ER20-M14	6/18/2008	498	NA	NA	NA	9.48	10.64	10.59	4.37	4.90	6.81E-03	7.64E-03	1.80E-02	2.02E-02	0.79	0.79	0.00

ER3-L	Collection Date	Time (days)	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase5)	SI (phase 3)
ER3-L1	2/13/2007	7	NA	NA	NA	9.16	10.32	11.47	0.00	0.00	8.00E-02	8.97E-02	2.15E-02	2.41E-02	1.21		
ER3-L2	2/13/2007	7	NA	NA	NA	9.13	10.29	11.44	0.00	0.00	1.97E-02	2.22E-02	2.08E-02	2.33E-02	0.55		
ER3-L3	3/2/2007	24	NA	NA	NA	9.76	10.92	12.07	4.64	5.20	2.89E-03	3.25E-03	1.97E-02	2.21E-02	0.97	1.08	0.11
ER3-L4	3/2/2007	24	NA	NA	NA	9.74	10.90	12.05	4.72	5.29	2.81E-03	3.15E-03	1.95E-02	2.19E-02	0.92	0.95	0.03
ER3-L5	3/28/2007	50	NA	NA	NA	10.40	11.56	12.71	5.04	5.65	NA		1.85E-02	2.07E-02			
ER3-L6	3/28/2007	50	NA	NA	NA	10.40	11.56	12.71	4.95	5.55	NA		1.94E-02	2.17E-02			
ER3-L7	5/30/2007	113	NA	NA	NA	10.98	12.14	13.29	5.00	5.61	NA		1.68E-01	1.88E-01			
ER3-L8	5/30/2007	113	NA	NA	NA	10.98	12.14	13.29	5.52	6.19	NA		1.53E-01	1.72E-01			
ER3-L9	2/12/2008	371	NA	NA	NA	9.97	11.13	12.28	5.03	5.65	1.90E-01	2.13E-01	1.41E-01	1.58E-01	3.21	7.62	4.41
ER3-L10	2/12/2008	371	NA	NA	NA	9.79	10.95	12.10	4.82	5.40	1.85E-01	2.08E-01	1.40E-01	1.57E-01	2.84	6.67	3.83

1							molarity to molality 1.1275	H+ log gamma 1.1131	A (pH correction 1.224		Cl- log gamma -0.2758		Mg++ log gamma 1.1781		aw 0.720915		Brucite log k 17.1090	Phase 5 log k 43.1900	Phase 3 log k 26.0297
GW20-M	Collection Date	Time (day)	Not Used	Not Used	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase-5)	SI (phase-3)
GW20-M1	2/13/2007	7	NA	NA	NA	NA	NA	7.46	8.68	8.63	NA		NA		0.01	0.01			
GW20-M2	2/13/2007	7	NA	NA	NA	NA	NA	7.44	8.66	8.61	NA		NA		0.01	0.01			
GW20-M3	3/2/2007	24	NA	NA	NA	NA	NA	7.94	9.16	9.11	4.93	5.55	0.86	0.97	0.01	0.01	-0.23	-0.52	-0.29
GW20-M4	3/2/2007	24	NA	NA	NA	NA	NA	7.92	9.14	9.09	5.03	5.67	0.82	0.92	0.01	0.01	-0.29	-0.67	-0.38
GW20-M5	3/28/2007	50	NA	NA	NA	NA	NA	8.11	9.33	9.28	5.34	6.02	NA		0.01	0.02			
GW20-M6	3/28/2007	50	NA	NA	NA	NA	NA	8.09	9.31	9.26	5.01	5.65	NA		0.01	0.02			
GW20-M7	5/30/2007	113	NA	NA	NA	NA	NA	8.24	9.46	9.41	4.99	5.63	NA		0.02	0.02			
GW20-M8	5/30/2007	113	NA	NA	NA	NA	NA	8.26	9.48	9.43	5.07	5.71	NA		0.01	0.02			
GW20-M9	8/23/2007	198	NA	NA	NA	NA	NA	8.38	9.60	9.55	5.11	5.76	1.12	1.26	0.02	0.02	0.76	2.04	1.28
GW20-M10	8/23/2007	198	NA	NA	NA	NA	NA	8.39	9.61	9.56	5.01	5.65	1.13	1.27	0.02	0.02	0.79	2.09	1.31
GW20-M11 (flake)	2/12/2008	371	NA	NA	NA	NA	NA	8.34	9.56	9.51	5.28	5.95	1.07	1.21	0.03	0.03	0.66	1.80	1.14
GW20-M12	2/12/2008	371	NA	NA	NA	NA	NA	8.35	9.57	9.52	5.03	5.67	1.03	1.16	0.02	0.03	0.67	1.78	1.11

3								H+ log gomma 1.0171			Cl- log gamma -0.2741		Mg++ log gamma 0.9926		aw 0.737546				
GW3S	Collection Date	Time (days)	Not Used	Not Used	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase-5)	SI (phase-3)
GW3-S1	2/13/2007	7	NA	NA	NA	NA	NA	7.85	9.07	9.02	NA		NA		0.02	0.02			
GW3-S2	2/13/2007	7	NA	NA	NA	NA	NA	8.00	9.22	9.17	NA		NA		NA				
GW3-S3	3/2/2007	24	NA	NA	NA	NA	NA	8.40	9.62	9.57	3.32	3.74	0.72	0.82	0.02	0.02	0.64	1.40	0.76
GW3-S4	3/2/2007	24	NA	NA	NA	NA	NA	8.34	9.56	9.51	3.33	3.75	0.67	0.76	0.02	0.02	0.49	1.01	0.52
GW3-S5	3/19/2007	41	NA	NA	NA	NA	NA	8.39	9.61	9.56	NA		0.64	0.73	0.01	0.02	0.57		
GW3-S6	3/19/2007	41	NA	NA	NA	NA	NA	8.38	9.60	9.55	NA		0.57	0.65	0.02	0.02	0.50		
GW3-S7	3/28/2007	50	NA	NA	NA	NA	NA	8.34	9.56	9.51	5.47	6.17	NA		0.02	0.02			
GW3-S8	3/28/2007	50	NA	NA	NA	NA	NA	8.34	9.56	9.51	5.17	5.83	NA		0.02	0.02			
GW3-S9 (wet ground)	4/16/2007	69	NA	NA	NA	NA	NA	8.38	9.60	9.55	NA		NA		0.02	0.02			
GW3-S10	4/16/2007	69	NA	NA	NA	NA	NA	8.37	9.59	9.54	NA		0.72	0.81	0.02	0.02	0.58		
GW3-S11	5/30/2007	113	NA	NA	NA	NA	NA	8.35	9.57	9.52	5.26	5.93	0.72	0.82	0.02	0.02	0.54	1.36	0.81
GW3-S12	5/30/2007	113	NA	NA	NA	NA	NA	8.36	9.58	9.53	5.15	5.80	0.71	0.80	0.02	0.02	0.55	1.36	0.81
GW3-S13	8/23/2007	198	NA	NA	NA	NA	NA	8.39	9.61	9.56	4.85	5.47	0.88	1.00	0.02	0.02	0.71	1.78	1.07
GW3-S14	8/23/2007	198	NA	NA	NA	NA	NA	8.39	9.61	9.56	5.08	5.73	0.88		0.02	0.02			
GW3-S15	12/11/2007	308	NA	NA	NA	NA	NA	8.39	9.61	9.56	5.46	6.15	0.84	0.95	0.01	0.02	0.69	1.77	1.08
GW3-S16	12/11/2007	308	NA	NA	NA	NA	NA	8.36	9.58	9.53	5.24	5.91	0.88	0.99	0.02	0.02	0.64	1.65	1.01
GW3-S17	6/18/2008	498	NA	NA	NA	NA	NA	8.30	9.52	9.47	6.13	6.91	0.79	0.89	0.02	0.03	0.48	1.28	0.81
GW3-S18	6/18/2008	498	NA	NA	NA	NA	NA	8.39	9.61	9.56	5.03	5.67	0.65	0.74	0.02	0.02	0.57	1.40	0.82

Constants:

Molarity to molality conversion factor for GWB in cell AR5 or AR29 = Concentration of Na+ (mol/l) / Concentration of Na+ (mol/kg), given in SP20-4 Appendix B = 3.98/3.53
For the H+ log gamma in AS5 or AS29, see the explanation section of worksheet "Fig 31" of this Excel file.
The pH correction factor A in cell AT5 can be found in Excel file "Brine acid base titration", worksheet "sum"
For the Cl- log gamma in AV5/29 see the explanation section of worksheet "Fig 31" of this Excel file
For the Mg++ log gamma in AX5/29, see the explanation section of worksheet "Fig 31" of this Excel file.
For the activity of water (aw) in AZ5/29 see the explanation section of worksheet "Fig 31" of this Excel file.
log k for brucite in cell BB5 = 17.1090
log k for phase-5 in cell BC5 = 43.19
log k for phase-3 in cell BD5 = 26.0297
These Log K's can be found in the EQ3/6 database: data0.hmo, and in the memo: Xiong et al., 2009

Calculation:

Time in column AM= collection date in column AL - starting date in cell A6 (data in column AL and cell A6 can be found in WIPP-MMMgO-5, p60-71)
Columns AN through AR are not used in the report.
pH in column AS can be found in notebook WIPP-MM MgO-5, p60-71.
pcH in column AT= pH in column AS + A (pH correction factor) in Cell AT5
pmH in column AU = pcH in column AT + log (molarity to malality conversion factor in Cell AR5)
Cl concentration (mole/l) in column AV can be found in Excel file "Cl analysis" on column D.
Cl concentration (mol/kg) in column AW = Cl concentration (mol/l) in column AV x molarity to molality conversion factor in cell AR5
Mg concentration (mol/l) in column AX can be found in excell file "ICP-AES" column G.
Mg Concentration (mol/kg) in column AY = Mg concentratin (mol/l) in column AV x molarity to molality conversion factor in cell AR5
Ca concentration (mol/l) in column AZ can be found in excell file "ICP-AES" column H.
Ca concentration (mol/kg) in column BA = Ca concentration (mol/l) in column AZ x molarity to molality conversion factor in cell AR5

SI of brucie in column BB = equation 8 in report
"=log (Mg concentration in column AY) + Mg log gamma in cell AX5/29 + 2 pmH in column AU - 2 H log gamma in cell AS5/29
+ 2 log Aw in cell AZ5/29 - log k of brucite in cell BB5

SI of phase-5 in column BC = equation 6 in report
"=3 log (Mg concentration in column AY) + 3 Mg log gamma in cell AX5/29 + 5 pmH in column AU
"- 5 H log gamma in cell AS5/29+ 9 log Aw in cell AZ5/29"
"+ log (Cl -IC in column AW) + Cl log gomma in cell AV5/29 - log k of phase-5 in cell BC5"

SI of phase-3 in column BD = equation 6 in report
"=2 log (Mg concentration in column AY) + 2 Mg log gamma in cell AX5/29 + 3 pmH in column AU"
"- 3 H log gamma in cell AS5/29+ 7 log Aw in cell AZ5/29"
"+ log (Cl concentration in column AW) + Cl log gamma in cell AV5/29 -log k of phase-3 in cell BD5"

3

GW20-L	Collection Date	Time (day)	Not Used	Not Used	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase-5)	SI (phase-3)
GW20-L1	2/13/2007	7	NA	NA	NA	NA	NA	7.30	8.52	8.47	0.00	0.00	NA		0.0129	0.0145			
GW20-L2	2/13/2007	7	NA	NA	NA	NA	NA	7.33	8.55	8.50	0.00	0.00	NA		0.0132	0.0148			
GW20-L3	3/2/2007	24	NA	NA	NA	NA	NA	7.54	8.76	8.71	5.22	5.88	NA		0.0000	0.0000			
GW20-L4	3/2/2007	24	NA	NA	NA	NA	NA	7.60	8.82	8.77	9.43	10.64	NA		0.0000	0.0000			
GW20-L5	3/28/2007	50	NA	NA	NA	NA	NA	7.79	9.01	8.96	5.67	6.39	NA		0.0139	0.0157			
GW20-L6	3/28/2007	50	NA	NA	NA	NA	NA	7.78	9.00	8.95	5.66	6.39	NA		0.0138	0.0155			
GW20-L7	5/30/2007	113	NA	NA	NA	NA	NA	8.07	9.29	9.24	5.11	5.76	NA		0.0158	0.0178			
GW20-L8	5/30/2007	113	NA	NA	NA	NA	NA	8.06	9.28	9.23	5.11	5.76	NA		0.0171	0.0193			
GW20-L9	8/23/2007	198	NA	NA	NA	NA	NA	8.32	9.54	9.49	4.69	5.28	1.20	1.35	0.0163	0.0184	0.67	1.79	1.12
GW20-L10	8/23/2007	198	NA	NA	NA	NA	NA	8.31	9.53	9.48	5.07	5.72	1.20	1.36	0.0168	0.0190	0.65	1.78	1.13
GW20-L11	2/12/2008	371	NA	NA	NA	NA	NA	8.34	9.56	9.51	4.62	5.21	1.03	1.16	0.0239	0.0270	0.65	1.69	1.04
GW20-L12	2/12/2008	371	NA	NA	NA	NA	NA	8.35	9.57	9.52	4.99	5.63	1.13	1.27	0.0247	0.0279	0.71	1.90	1.19

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GW3-M	Collection Date	Time (days)	Not Used	Not Used	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase-5)	SI (phase-3)
GW3-M1	2/13/2007	7	NA	NA	NA	NA	NA	7.85	9.07	9.02	NA		0.91	1.02	0.0143	0.0161	-0.36		
GW3-M2	2/13/2007	7	NA	NA	NA	NA	NA	8.00	9.22	9.17	NA		0.89	1.00	0.0148	0.0167	-0.07		
GW3-M3	3/2/2007	24	NA	NA	NA	NA	NA	8.40	9.62	9.57	5.16	5.81	0.79	0.89	0.1526	0.1721	0.68	1.71	1.03
GW3-M4	3/2/2007	24	NA	NA	NA	NA	NA	8.34	9.56	9.51	5.34	6.02	NA		0.1846	0.2082			
GW3-M5	3/28/2007	50	NA	NA	NA	NA	NA	8.39	9.61	9.56	4.87	5.50	0.84	0.94	0.0152	0.0172	0.68	1.71	1.03
GW3-M6	3/28/2007	50	NA	NA	NA	NA	NA	8.38	9.60	9.55	5.46	6.16	0.78	0.88	0.0140	0.0158	0.63	1.62	0.99
GW3-M7	5/30/2007	113	NA	NA	NA	NA	NA	8.39	9.61	9.56	4.86	5.48	0.76	0.86	0.0181	0.0204	0.64	1.58	0.94
GW3-M8	5/30/2007	113	NA	NA	NA	NA	NA	8.37	9.59	9.54	4.90	5.53	0.70	0.78	0.0162	0.0183	0.56	1.37	0.81
GW3-M9	8/23/2007	198	NA	NA	NA	NA	NA	8.47	9.69	9.64	4.85	5.46	0.78	0.87	0.0170	0.0192	0.81	2.01	1.20
GW3-M10	8/23/2007	198	NA	NA	NA	NA	NA	8.43	9.65	9.60	0.00	0.00	0.78	0.87	0.0172	0.0194	0.73		
GW3-M11	12/11/2007	308	NA	NA	NA	NA	NA	8.36	9.58	9.53	5.33	6.01	0.77	0.86	0.0152	0.0171	0.58	1.48	0.90
GW3-M12	12/11/2007	308	NA	NA	NA	NA	NA	8.37	9.59	9.54	5.26	5.93	0.76	0.85	0.0156	0.0176	0.60	1.51	0.91
GW3-M13	6/18/2008	498	NA	NA	NA	NA	NA	8.31	9.53	9.48	4.44	5.00	0.59	0.67	0.0186	0.0210	0.37	0.82	0.44
GW3-M14	6/18/2008	498	NA	NA	NA	NA	NA	8.35	9.57	9.52	5.92	6.67	0.68	0.77	0.0216	0.0243	0.51	1.33	0.81

1						log 0.04885684	molarity to molality coversion factor 1.1191	H+ log gamma 1.0935	A (pH correction factor) 1.2060		Cl- log gamma -0.2733		Mg++ log gamma 1.1803		aw 0.732274		Brucite log k 17.1090	Phase 5 log k 43.1900	Phase 3 log k 26.0297
MgCL20-M	Collection Date	Time (day)	Not Used	Not Used	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase-5)	SI (phase-3)
MgCL20-M1	2/13/2007	7	NA	NA	NA	NA	NA	8.18	9.39	9.34	NA		NA		0.0049	0.0055			
MgCL20-M2	2/13/2007	7	NA	NA	NA	NA	NA	8.18	9.39	9.34	NA		NA		0.0045	0.0051			
MgCL20-M3	3/2/2007	24	NA	NA	NA	NA	NA	8.16	9.37	9.32	NA		0.82	0.92	0.0047	0.0053	0.21		
MgCL20-M4	3/2/2007	24	NA	NA	NA	NA	NA	8.18	9.39	9.34	NA		0.85	0.96	0.0048	0.0054	0.27		
MgCL20-M5	3/19/2007	41	NA	NA	NA	NA	NA	8.12	9.33	9.28	NA		0.66	0.74	0.0048	0.0054	0.04		
MgCL20-M6	3/19/2007	41	NA	NA	NA	NA	NA	8.13	9.34	9.29	NA		NA		0.0049	0.0055			
MgCL20-M7	3/28/2007	50	NA	NA	NA	NA	NA	8.10	9.31	9.26	5.54	6.20	NA		0.0053	0.0060			
MgCL20-M8	3/28/2007	50	NA	NA	NA	NA	NA	8.09	9.30	9.25	6.07	6.79	NA		0.0056	0.0062			
MgCL20-M9 (soak over night)	4/16/2007	69	NA	NA	NA	NA	NA	8.11	9.32	9.27	NA		NA		0.0053	0.0059			
MgCL20-M10	4/16/2007	69	NA	NA	NA	NA	NA	8.09	9.30	9.25	NA		NA		0.0059	0.0066			
MgCL20-M11	5/30/2007	113	NA	NA	NA	NA	NA	8.09	9.30	9.25	5.39	6.03	NA		0.0052	0.0059			
MgCL20-M12	5/30/2007	113	NA	NA	NA	NA	NA	8.13	9.34	9.29	5.55	6.21	NA		0.0050	0.0056			
MgCL20-M13	7/16/2007	160	NA	NA	NA	NA	NA	8.13	9.34	9.29	5.99	6.70	0.90	1.01	0.0167	0.0187	0.19	0.67	0.48
MgCL20-M14	7/16/2007	160	NA	NA	NA	NA	NA	8.14	9.35	9.30	6.14	6.87	0.78	0.87	0.0169	0.0189	0.15	0.53	0.39
MgCl20M-15	8/23/2007	198	NA	NA	NA	NA	NA	8.17	9.38	9.33	4.57	5.12	0.96	1.07	0.0055	0.0061	0.30	0.82	0.53
MgCl20M-16	8/23/2007	198	NA	NA	NA	NA	NA	8.18	9.39	9.34	4.86	5.44	1.03	1.15	0.0057	0.0063	0.35	1.00	0.65
MgCl20M-17	12/11/2007	308	NA	NA	NA	NA	NA	8.19	9.40	9.35	5.91	6.61	1.10	1.23	0.0065	0.0073	0.40	1.22	0.83
MgCl20M-18	12/11/2007	308	NA	NA	NA	NA	NA	8.22	9.43	9.38	5.70	6.38	1.09	1.22	0.0504	0.0564	0.45	1.34	0.89
MgCl20M19	4/17/2008	436	NA	NA	NA	NA	NA	8.17	9.38	9.33	5.32	5.95	1.09	1.22	0.0063	0.0071	0.35	1.06	0.71
MgCl20M20	4/17/2008	436	NA	NA	NA	NA	NA	8.16	9.37	9.32	5.20	5.82	1.08	1.21	0.0062	0.0069	0.33	0.99	0.66
3								H+ log gomma 0.9825	A(pH correction factor) 1.2060		Cl- log gomma -0.2706		Mg++ log gomma 0.9747		aw 0.752603				
MgCL3-S	Collection Date	Time (day)	Not Used	Not Used	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase-5)	SI (phase-3)
MgCL3-S1	2/13/2007	7	NA	NA	NA	NA	NA	8.32	9.53	9.48	NA		NA		0.0307	0.0344			
MgCL3-S2	2/13/2007	7	NA	NA	NA	NA	NA	8.31	9.52	9.47	NA		NA		0.0316	0.0353			
MgCL3-S3	3/2/2007	24	NA	NA	NA	NA	NA	8.34	9.55	9.50	5.65	6.33	NA		0.0343	0.0383			
MgCL3-S4	3/2/2007	24	NA	NA	NA	NA	NA	8.35	9.56	9.51	NA		0.60	0.67	0.0350	0.0392	0.49		
MgCL3-S5	3/19/2007	41	NA	NA	NA	NA	NA	8.24	9.45	9.40	5.74	6.43	0.46	0.51	0.0360	0.0403	0.16	0.36	0.21
MgCL3-S6	3/19/2007	41	NA	NA	NA	NA	NA	8.24	9.45	9.40	NA		0.36	0.40	0.0360	0.0403	0.05		
MgCL3-S7	3/28/2007	50	NA	NA	NA	NA	NA	8.25	9.46	9.41	5.32	5.96	NA		0.0394	0.0441			
MgCL3-S8	3/28/2007	50	NA	NA	NA	NA	NA	8.25	9.46	9.41	5.17	5.79	NA		0.0405	0.0454			
MgCL3-S9 (wet ground)	4/16/2007	69	NA	NA	NA	NA	NA	8.23	9.44	9.39	NA		NA		0.0433	0.0485			
MgCL3-S10	4/16/2007	69	NA	NA	NA	NA	NA	8.23	9.44	9.39	NA		NA		0.0501	0.0560			
MgCL3-S11	5/30/2007	113	NA	NA	NA	NA	NA	8.21	9.42	9.37	5.20	5.82	NA		0.0455	0.0509			
MgCl3-S12	5/30/2007	113	NA	NA	NA	NA	NA	8.21	9.42	9.37	5.18	5.80	NA		0.0470	0.0526			
MgCL3-S13	7/16/2007	160	NA	NA	NA	NA	NA	8.32	9.53	9.48	5.65	6.33	0.57	0.64	0.0663	0.0742	0.41	1.04	0.63
NA	NA		NA	NA	NA	NA	NA	NA	NA	NA	NA		NA		NA				
MgCl3-S15	8/23/2007	198	NA	NA	NA	NA	NA	8.28	9.49	9.44	5.51	6.17	0.76	0.85	0.0539	0.0604	0.46	1.20	0.75
MgCl3-S16	8/23/2007	198	NA	NA	NA	NA	NA	8.28	9.49	9.44	5.22	5.85	0.75	0.84	0.0531	0.0594	0.45	1.17	0.72
MgCl3-S17	12/11/2007	308	NA	NA	NA	NA	NA	8.15	9.36	9.31	5.54	6.20	0.75	0.84	0.0502	0.0561	0.19	0.54	0.35
MgCl3-S18	12/11/2007	308	NA	NA	NA	NA	NA	8.14	9.35	9.30	5.64	6.31	0.79	0.88	0.0057	0.0064	0.19	0.56	0.37
MgCl3-S19	4/17/2008	436	NA	NA	NA	NA	NA	8.16	9.37	9.32	5.36	6.00	0.86	0.96	0.0513	0.0574	0.27	0.75	0.48
MgCl3-S20	4/17/2008	436	NA	NA	NA	NA	NA	8.19	9.40	9.35	5.40	6.04	0.81	0.91	0.0473	0.0530	0.30	0.83	0.52
MgCl3-S21	6/18/2008	498	NA	NA	NA	NA	NA	8.14	9.35	9.30	5.48	6.13	0.71	0.79	0.0597	0.0668	0.15	0.41	0.27
MgCl3-S22	6/18/2008	498	NA	NA	NA	NA	NA	8.15	9.36	9.31	5.19	5.81	0.70	0.79	0.0574	0.0642	0.17	0.43	0.27

Constants:

Molarity to molality conversion factor for simplified GWB in cell CF5 can be found in Excel file "MgO in brine", data sheet "SGWB"
For the H+ log gamma in CG5 or CG29 see the explanation section of worksheet "Fig 32" of this Excel file
The pH correction factor A in cell CH5 can be found in the Excel file "Brine acid base titration", worksheet "sum"
For the Cl- log gamma in CJ5/29 see the explanation section of worksheet "Fig 32" of this Excel file
For the Mg++ log gamma in CL5/29 see the explanation section of worksheet "Fig 32" of this Excel file.
For the activity of water (aw) in CN5/29 see the explanation section of worksheet "Fig 32" of this Excel file.
log k for brucite in cell CP5 = 17.1090
log k for phase-5 in cell CQ5 = 43.19
log k for phase-3 in cell CR5 = 26.0297
These Log K's can be found in the EQ3/6 database: data0.hmo, and in the memo: Xiong et al., 2009

Calculation:

Time in column CA = collection date in column BZ - starting date in cell A6 (data in column BZ and cell A6 can be found in WIPP-MMMgO-5, p60-71)
Columns CB through CF are not used in the report
pH in column CG can be found in notebook WIPP-MMMgO-5, p60-71.
pcH in column CH = pH in column CG + A (pH correction factor) in Cell CH5
pmH in column CI = pcH in column CH + log (molarity to molality conversion factor in Cell F5)
Cl concentration (mole/l) in column CJ can be found in Excel file "Cl analysis", column D.
Cl concentration (mol/kg) in column CK = Cl concentration (mol/l) in column CJ x molar conversion factor in cell CF5
Mg concentration (mol/l) in column CL can be found in excel file "ICP-AES" column G.
Mg concentration (mol/kg) in column CM = Mg concentration (mol/l) in column CL x molar conversion factor in cell CF5
Ca concentration (mol/l) in column CN can be found in excel file "ICP-AES" column H.
Ca concentration (mol/kg) in column CO = Ca concentration (mol/l) in column CN x molar conversion factor in cell CF5

SI of brucite in column P = equation 8 in report - log k of brucite
"=log (Mg concentration in column CM)+ Mg log gamma in cell CL5/29 + 2 pmH in column CI- 2 H log gamma in cell CG5/29
+ 2 log aw in cell CN5 - log k of brucite in cell CP5

SI of phase-5 in column CQ = equation 6 in report - log k of phase-5
"=3 log (Mg concentration mol/kg in column CM)+ 3 Mg log gamma in cell CL5/29 + 5 pmH in column CI
"- 5 H log gamma in cell CG5/29+ 9 log aw in cell CN5/29"
"+ log (Cl concentration in column CK) + Cl log gamma in cell CJ5/29 - log k of phase-5 in cell CQ5"

SI of phase-3 in column Q = equation 6 in report -long k of phase-3
"= 2 log (Mg concentration in column CM)+ 2 Mg log gamma in cell CL5/29 + 3 pmH in column CI
"- 3 H log gamma in cell CG5/29+ 7 log aw in cell CN5/29"
"+ log (Cl concentration in column CK) + Cl log gamma in cell CJ5/29 -log k of phase-3 in cell CR5"

2																					
MgCL20-L	Collection Date	Time (day)	Not Used	Not Used	Not Used	Not Used	Not Used	Not Used	Not Used	Not Used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase-5)	SI (phase-3)
MgCL20-L1	2/13/2007	7	NA	NA	NA	NA	NA	NA	NA	NA	8.21	9.42	9.37	NA		NA		0.0045	0.0050			
MgCL20-L2	2/13/2007	7	NA	NA	NA	NA	NA	NA	NA	NA	8.25	9.46	9.41	NA		NA		0.0066	0.0074			
MgCL20-L3	3/2/2007	24	NA	NA	NA	NA	NA	NA	NA	NA	8.11	9.32	9.27	NA		0.87	0.98	0.0047	0.0052	0.14		
MgCL20-L4	3/2/2007	24	NA	NA	NA	NA	NA	NA	NA	NA	8.17	9.38	9.33	NA		0.87	0.98	0.0045	0.0050	0.26		
MgCL20-L5	3/19/2007	41	NA	NA	NA	NA	NA	NA	NA	NA	8.12	9.33	9.28	NA		0.77	0.86	0.0045	0.0051	0.10		
MgCL20-L6	3/19/2007	41	NA	NA	NA	NA	NA	NA	NA	NA	8.09	9.30	9.25	NA		0.68	0.76	0.0046	0.0051	-0.01		
MgCL20-L7	3/28/2007	50	NA	NA	NA	NA	NA	NA	NA	NA	8.12	9.33	9.28	5.47	6.12	NA		0.0055	0.0062			
MgCL20-L8	3/28/2007	50	NA	NA	NA	NA	NA	NA	NA	NA	8.14	9.35	9.30	5.19	5.81	NA		0.0050	0.0056			
MgCL20-L9(wet ground)	4/16/2007	69	NA	NA	NA	NA	NA	NA	NA	NA	8.11	9.32	9.27	NA		NA		0.0052	0.0058			
MgCL20-L10	4/16/2007	69	NA	NA	NA	NA	NA	NA	NA	NA	8.08	9.29	9.24	NA		NA		0.0053	0.0059			
MgCL20-L11	5/30/2007	113	NA	NA	NA	NA	NA	NA	NA	NA	8.09	9.30	9.25	5.62	6.29	NA		0.0054	0.0060			
MgCL20-L12	5/30/2007	113	NA	NA	NA	NA	NA	NA	NA	NA	8.11	9.32	9.27	5.28	5.90	NA		0.0053	0.0059			
MgCL20-L13	7/16/2007	160	NA	NA	NA	NA	NA	NA	NA	NA	8.12	9.33	9.28	5.94	6.65	0.93	1.04	0.0169	0.0189	0.19	0.66	0.47
MgCL20-L14	7/16/2007	160	NA	NA	NA	NA	NA	NA	NA	NA	8.07	9.28	9.23	5.94	6.65	0.88	0.99	0.0171	0.0191	0.06	0.34	0.28
MgCL20-L15	8/23/2007	198	NA	NA	NA	NA	NA	NA	NA	NA	8.15	9.36	9.31	5.27	5.89	1.24	1.39	0.0060	0.0067	0.37	1.12	0.76
MgCL20-L16	8/23/2007	198	NA	NA	NA	NA	NA	NA	NA	NA	8.14	9.35	9.30	5.31	5.94	1.16	1.30	0.0063	0.0071	0.32	0.99	0.67
MgCL20-L17	12/11/2007	308	NA	NA	NA	NA	NA	NA	NA	NA	8.15	9.36	9.31	5.58	6.24	1.12	1.25	0.0060	0.0067	0.33	1.02	0.70
MgCL20-L18	12/11/2007	308	NA	NA	NA	NA	NA	NA	NA	NA	8.14	9.35	9.30	5.65	6.32	1.12	1.25	0.0053	0.0059	0.31	0.97	0.67
MgCL20-L19	4/17/2008	436	NA	NA	NA	NA	NA	NA	NA	NA	8.15	9.36	9.31	5.35	5.99	1.15	1.29	0.0062	0.0070	0.34	1.03	0.70
MgCL20-L20	4/17/2008	436	NA	NA	NA	NA	NA	NA	NA	NA	8.16	9.37	9.32	5.51	6.17	1.14	1.27	0.0058	0.0065	0.35	1.08	0.73

4																					
MgCL3-M	Collection Date	Time (day)	Not used	Not used	Not used	Not used	Not used	Not used	Not used	Not used	pH	pcH	pmH	Cl concentration (mol/l)	Cl concentration (mol/kg)	Mg concentration (mol/l)	Mg concentration (mol/kg)	Ca concentration (mol/l)	Ca concentration (mol/kg)	SI (brucite)	SI (phase-5)	SI (phase-3)
MgCL3-M1	2/13/2007	7	NA	NA	NA	NA	NA	NA	NA	NA	8.25	9.46	9.41	NA		NA		0.03	0.04			
MgCL3-M2	2/13/2007	7	NA	NA	NA	NA	NA	NA	NA	NA	8.24	9.45	9.40	NA		NA		0.03	0.04			
MgCL3-M3	3/2/2007	24	NA	NA	NA	NA	NA	NA	NA	NA	8.28	9.49	9.44	5.57	6.23	0.71	0.80	0.03	0.04	0.43	1.13	0.70
MgCL3-M4	3/2/2007	24	NA	NA	NA	NA	NA	NA	NA	NA	8.29	9.50	9.45	5.33	5.96	0.74	0.83	0.03	0.04	0.47	1.21	0.75
MgCL3-M5	3/19/2007	41	NA	NA	NA	NA	NA	NA	NA	NA	8.18	9.39	9.34	NA		0.52	0.59	0.03	0.04	0.10		
MgCL3-M6	3/19/2007	41	NA	NA	NA	NA	NA	NA	NA	NA	8.17	9.38	9.33	NA		0.50	0.56	0.03	0.04	0.06		
MgCL3-M7	3/28/2007	50	NA	NA	NA	NA	NA	NA	NA	NA	8.20	9.41	9.36	5.21	5.83	NA		0.04	0.05			
MgCL3-M8	3/28/2007	50	NA	NA	NA	NA	NA	NA	NA	NA	8.17	9.38	9.33	5.16	5.77	NA		0.04	0.05			
MgCL3-M9	4/16/2007	69	NA	NA	NA	NA	NA	NA	NA	NA	8.16	9.37	9.32	NA		0.69	0.78	0.05	0.05	0.18		
MgCL3-M10	4/16/2007	69	NA	NA	NA	NA	NA	NA	NA	NA	8.16	9.37	9.32	NA		0.63	0.71	0.04	0.05	0.14		
MgCL3-M11	5/30/2007	113	NA	NA	NA	NA	NA	NA	NA	NA	8.16	9.37	9.32	5.25	5.88	0.65	0.73	0.05	0.05	0.15	0.39	0.24
MgCL3-M12	5/30/2007	113	NA	NA	NA	NA	NA	NA	NA	NA	8.16	9.37	9.32	5.45	6.10	0.69	0.77	0.05	0.06	0.17	0.47	0.30
MgCL3-M13	7/16/2007	160	NA	NA	NA	NA	NA	NA	NA	NA	8.26	9.47	9.42	9.78	10.94	0.67	0.75	0.06	0.07	0.36	1.19	0.83
NA			NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA		NA		NA				
MgCL3-M15	8/23/2007	198	NA	NA	NA	NA	NA	NA	NA	NA	8.26	9.47	9.42	5.47	6.12	0.85	0.95	0.05	0.06	0.46	1.24	0.78
MgCL3-M16	8/23/2007	198	NA	NA	NA	NA	NA	NA	NA	NA	8.26	9.47	9.42	5.34	5.97	0.86	0.96	0.05	0.06	0.47	1.25	0.78
MgCL3-M17	12/11/2007	308	NA	NA	NA	NA	NA	NA	NA	NA	8.19	9.40	9.35	5.47	6.12	0.85	0.95	0.05	0.06	0.32	0.89	0.57
MgCL3-M18	12/11/2007	308	NA	NA	NA	NA	NA	NA	NA	NA	8.22	9.43	9.38	5.43	6.07	0.82	0.92	0.05	0.05	0.37	1.00	0.63
MgCl3-M19	4/17/2008	436	NA	NA	NA	NA	NA	NA	NA	NA	8.16	9.37	9.32	5.39	6.03	0.91	1.02	0.05	0.06	0.30	0.83	0.54
MgCl3-M20	4/17/2008	436	NA	NA	NA	NA	NA	NA	NA	NA	8.19	9.40	9.35	5.40	6.05	0.85	0.95	0.05	0.06	0.33	0.89	0.57
MgCl3-M21	6/18/2008	498	NA	NA	NA	NA	NA	NA	NA	NA	8.15	9.36	9.31	5.53	6.18	0.69	0.77	0.06	0.07	0.15	0.42	0.27
MgCl3-M22	6/18/2008	498	NA	NA	NA	NA	NA	NA	NA	NA	8.18	9.39	9.34	5.58	6.25	0.64	0.72	0.06	0.07	0.19	0.49	0.31

	Sample name (dilution factor)	Cl concentration (ppm)	Cl concentration (mol/l)	Analysis Date	Scientific Notebook and pg.
1					
2					
3	ER20M3 (1:10000)	15.5238	4.38	7/1/2008	Wipp-mmmgo-11, p15
4	ER20M4 (1:10000)	15.44	4.36	7/1/2008	Wipp-mmmgo-11, p15
5	ER20M5 (1:10000)	17.1338	4.83	7/14/2008	Wipp-mmmgo-11, p22
6	ER20M6 (1:10000)	16.7456	4.72	7/14/2008	Wipp-mmmgo-11, p22
7	ER20M7 (1:10000)	16.5761	4.68	7/1/2008	Wipp-mmmgo-11, p15
8	ER20M8 (1:10000)	16.2326	4.58	7/17/2008	Wipp-mmmgo-11, p24
9	ER20M9 (1:10000)	18.0129	5.08	7/23/2008	Wipp-mmmgo-11, p27
10	ER20M10 (1:10000)	15.3391	4.33	7/23/2008	Wipp-mmmgo-11, p27
11	ER20M11 (1:10000)	16.6301	4.69		
12	ER20M12 (1:10000)	16.5533	4.67		
13					
14	ER20M14(1:10000)	15.4764	4.37	6/23/2008	Wipp-mmmgo-11, p15
15					
16					

ER20M11 (1:10000)	17.0534	4.81	7/3/2008	Wipp-mmmgo-11, p19
ER20M11 (1:10000)	16.2069	4.57	8/4/2008	Wipp-mmmgo-11, p31
ER20M12 (1:10000)	16.9747	4.79	7/3/2008	Wipp-mmmgo-11, p19
ER20M12 (1:10000)	16.1320	4.55	8/4/2008	Wipp-mmmgo-11, p31

1					
2					
3					
4					
5					
6					
7	ER20S7 (1:10000)	16.1112	4.54	7/16/2008	Wipp-mmmgo-11, p23
8	ER20S8 (1:10000)	15.3980	4.34	7/16/2008	Wipp-mmmgo-11, p23
9					
10					
11	ER20S11 (1:10000)	15.9946	4.51	7/21/2008	Wipp-mmmgo-11, p25
12	ER20S12 (1:10000)	15.8960	4.48	7/21/2008	Wipp-mmmgo-11, p25
13	ER20S13 (1:10000)	16.0836	4.54	7/23/2008	Wipp-mmmgo-11, p27
14	ER20S14 (1:10000)	14.6220	4.12	7/23/2008	Wipp-mmmgo-11, p27
15	ER20S15 (1:10000)	16.5560	4.67		
16	ER20S16 (1:10000)	16.7132	4.71		
17	ER20S17(1:10000)	15.6392	4.41	6/23/2008	Wipp-mmmgo-11, p15
18	ER20S18 (1:10000)	15.4919	4.37	6/23/2008	Wipp-mmmgo-11, p15

ER20S16 (1:10000)	17.0355	4.81	7/7/2008	Wipp-mmmgo-11, p20
ER20S16 (1:10000)	16.3910	4.62	7/31/2008	Wipp-mmmgo-11, p30
ER20S15 (1:10000)	17.0840	4.82	7/7/2008	Wipp-mmmgo-11, p20
ER20S15 (1:10000)	16.0281	4.52	7/31/2008	Wipp-mmmgo-11, p30

1					
2					
3	ER3L3 (1:10000)	16.4446	4.64	7/9/2008	Wipp-mmmgo-11, p21
4	ER3L4 (1:10000)	16.7268	4.72	7/9/2008	Wipp-mmmgo-11, p21
5	ER3L5 (1:10000)	17.8658	5.04	7/14/2008	Wipp-mmmgo-11, p22
6	ER3L6 (1:10000)	17.5376	4.95	7/14/2008	Wipp-mmmgo-11, p22
7	ER3L7 (1:10000)	17.7174	5.00	7/1/2008	Wipp-mmmgo-11, p15
8	ER3L8 (1:10000)	19.5652	5.52	7/16/2008	Wipp-mmmgo-11, p23
9	ER3L9 (1:10000)	17.8458	5.03	8/5/2008	Wipp-mmmgo-11, p32
10	ER3L10 (1:10000)	17.0809	4.82	8/5/2008	Wipp-mmmgo-11, p32

1				
2				
3	ER3M3 (1:10000)	7.82135772	2.21	
4	ER3M4 (1:10000)	17.0402	4.81	7/9/2008 Wipp-mmmgo-11, p21
5	ER3M5 (1:10000)	17.8710	5.04	7/9/2008 Wipp-mmmgo-11, p21
6	ER3M6 (1:10000)	17.7160	5.00	7/9/2008 Wipp-mmmgo-11, p21
7	ER3M7 (1:10000)	15.8032	4.46	7/16/2008 Wipp-mmmgo-11, p23
8	ER3M8 (1:10000)	15.5885	4.40	7/16/2008 Wipp-mmmgo-11, p23
9	ER3M9 (1:10000)	16.0223	4.52	8/5/2008 Wipp-mmmgo-11, p32
10	ER3M10 (1:10000)	17.9236	5.06	8/5/2008 Wipp-mmmgo-11, p32

ER3M3 (1:10000)	7.9328	2.24	7/1/2008 Wipp-mmmgo-11, p15
ER3M3 (1:10000)	7.7099	2.17	7/22/2008 Wipp-mmmgo-11, p26

1				
2				
3	GW20L3 (1:10000)	18.4989	5.22	7/1/2008 Wipp-mmmgo-11, p15
4	GW20L4(1:10000)	33.4494	9.43	7/1/2008 Wipp-mmmgo-11, p15
5	GW20L5 (1:10000)	20.1066	5.67	7/14/2008 Wipp-mmmgo-11, p22
6	GW20L6(1:10000)	20.0790	5.66	7/14/2008 Wipp-mmmgo-11, p22
7	GW20L7 (1:10000)	18.1133	5.11	7/16/2008 Wipp-mmmgo-11, p23
8	GW20L8 (1:10000)	18.1262	5.11	7/16/2008 Wipp-mmmgo-11, p23
9	GW20L9 (1:10000)	16.6102	4.69	7/22/2008 Wipp-mmmgo-11, p26
10	GW20L10 (1:10000)	17.9887	5.07	7/22/2008 Wipp-mmmgo-11, p26
11	GW20L11 (1:10000)	16.3884	4.62	8/5/2008 Wipp-mmmgo-11, p32
12	GW20L12 (1:10000)	17.6949	4.99	8/5/2008 Wipp-mmmgo-11, p32

1				
2				
3	GW20M3 (1:10000)	17.4615	4.93	7/1/2008 Wipp-mmmgo-11, p15
4	GW20M4(1:10000)	17.8194	5.03	7/1/2008 Wipp-mmmgo-11, p15
5	GW20M5 (1:10000)	18.9309	5.34	7/14/2008 Wipp-mmmgo-11, p22
6	GW20M6 (1:10000)	17.7542	5.01	7/16/2008 Wipp-mmmgo-11, p23
7	GW20M7 (1:10000)	17.6925	4.99	7/16/2008 Wipp-mmmgo-11, p23
8	GW20M8 (1:10000)	17.9596	5.07	7/17/2008 Wipp-mmmgo-11, p24
9	GW20M9 (1:10000)	18.1227	5.11	7/22/2008 Wipp-mmmgo-11, p26
10	GW20M10 (1:10000)	17.7733	5.01	
11	GW20M11 (1:10000)	18.7197	5.28	8/5/2008 Wipp-mmmgo-11, p32
12	GW20M12 (1:10000)	17.8240	5.03	8/5/2008 Wipp-mmmgo-11, p32

GW2M10 (1:10000)	17.4570	4.92	7/23/2008 Wipp-mmmgo-11, p27
GW20M10 (1:10000)	18.0896	5.10	7/22/2008 Wipp-mmmgo-11, p26

1				
2				
3	GW3M3 (1:10000)	18.2818	5.16	7/9/2008 Wipp-mmmgo-11, p21
4	GW3M4 (1:10000)	18.9154	5.34	7/9/2008 Wipp-mmmgo-11, p21
5	GW3M5 (1:10000)	17.2814	4.87	7/16/2008 Wipp-mmmgo-11, p23
6	GW3M6 (1:10000)	19.3610	5.46	7/14/2008 Wipp-mmmgo-11, p22
7	GW3M7 (1:10000)	17.2170	4.86	7/16/2008 Wipp-mmmgo-11, p23
8	GW3M8 (1:10000)	17.3778	4.90	7/16/2008 Wipp-mmmgo-11, p23
9	GW3M9 (1:10000)	17.1791	4.85	7/23/2008 Wipp-mmmgo-11, p27
10				
11	GW3M11 (1:10000)	18.9136	5.33	
12	GW3M12 (1:10000)	18.6620	5.26	
13	GW3M13 (1:10000)	15.7262	4.44	6/23/2008 Wipp-mmmgo-11, p15
14	GW3M14 (1:10000)	20.9853	5.92	6/23/2008 Wipp-mmmgo-11, p15

GW3M11 (1:10000)	19.0256	5.37	7/3/2008 Wipp-mmmgo-11, p19
GW3M11 (1:10000)	18.8017	5.30	8/4/2008 Wipp-mmmgo-11, p31
GW3M12 (1:10000)	18.8431	5.32	7/3/2008 Wipp-mmmgo-11, p19
GW3M12 (1:10000)	18.4809	5.21	8/4/2008 Wipp-mmmgo-11, p31

1				
2				
3	GW3S3 (1:10000)	11.7645	3.32	7/22/2008 Wipp-mmmgo-11, p26
4	GW3S4 (1:10000)	11.7985	3.33	7/9/2008 Wipp-mmmgo-11, p21
5				
6				
7	GW3S7 (1:10000)	19.409	5.47	7/1/2008 Wipp-mmmgo-11, p15
8	GW3S8 (1:10000)	18.3368	5.17	7/17/2008 Wipp-mmmgo-11, p24
9				
10				
11	GW3S11 (1:10000)	18.6311	5.26	7/21/2008 Wipp-mmmgo-11, p25
12	GW3S12 (1:10000)	18.2527	5.15	7/21/2008 Wipp-mmmgo-11, p25
13	GW3S13 (1:10000)	17.2046	4.85	7/23/2008 Wipp-mmmgo-11, p27
14	GW3S14 (1:10000)	18.0208	5.08	7/23/2008 Wipp-mmmgo-11, p27
15	GW3S15 (1:10000)	19.3454	5.46	
16	GW3S16 (1:10000)	18.5945	5.24	
17	GW3S17 (1:10000)	21.7199	6.13	6/23/2008 Wipp-mmmgo-11, p15
18	GW3S18 (1:10000)	17.8228	5.03	6/23/2008 Wipp-mmmgo-11, p15

GW3S3 (1:10000)	[redacted]	0.59	7/9/2008 Wipp-mmmgo-11, p21
GW3S15 (1:10000)	20.2005	5.70	7/7/2008 Wipp-mmmgo-11, p20
GW3S15 (1:10000)	18.4903	5.22	7/31/2008 Wipp-mmmgo-11, p30
GW3S16 (1:10000)	17.9515	5.06	7/7/2008 Wipp-mmmgo-11, p20
GW3S16 (1:10000)	19.2376	5.43	7/31/2008 Wipp-mmmgo-11, p30

1					
2					
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5					
6					
7	MgCl2 20L7 (1:10000)	19.3883	5.47	7/17/2008	Wipp-mmmgo-11, p24
8	MgCl2 20L8 (1:10000)	18.4062	5.19	7/17/2008	Wipp-mmmgo-11, p24
9					
10					
11	MgCl2 20L11 (1:10000)	19.9269	5.62	7/21/2008	Wipp-mmmgo-11, p25
12	MgCl2 20L12 (1:10000)	18.7017	5.28	7/22/2008	Wipp-mmmgo-11, p26
13	MgCl2 20L13 (1:10000)	21.0637	5.94	7/3/2008	Wipp-mmmgo-11, p19
14	MgCl2 20L14 (1:10000)	21.0706	5.94	7/3/2008	Wipp-mmmgo-11, p19
15	MgCl2 20L15 (1:10000)	18.6738	5.27	7/22/2008	Wipp-mmmgo-11, p26
16	MgCl2 20L16 (1:10000)	18.8254	5.31	7/22/2008	Wipp-mmmgo-11, p26
17	MgCl2 20L17 (1:10000)	19.7805	5.58		
18	MgCl2 20L18 (1:10000)	20.0294	5.65		
19	MgCl2 20L19 (1:10000)	18.9710	5.35	8/4/2008	Wipp-mmmgo-11, p31
20	MgCl2 20L20 (1:10000)	19.5338	5.51	8/4/2008	Wipp-mmmgo-11, p31

MgCl2 20L17 (1:10000)	20.7288	5.85	7/7/2008	Wipp-mmmgo-11, p20
MgCl2 20L17 (1:10000)	18.8322	5.31	7/31/2008	Wipp-mmmgo-11, p30
MgCl2 20L18 (1:10000)	20.7462	5.85	7/7/2008	Wipp-mmmgo-11, p20
MgCl2 20L18 (1:10000)	19.3127	5.45	7/31/2008	Wipp-mmmgo-11, p30

1					
2					
3					
4					
5					
6					
7	MgCl2 20M7 (1:10000)	19.6543	5.54	7/1/2008	Wipp-mmmgo-11, p15
8	MgCl2 20M8 (1:10000)	21.5216	6.07	7/17/2008	Wipp-mmmgo-11, p24
9					
10					
11	MgCl2 20M11 (1:10000)	19.1033	5.39	7/21/2008	Wipp-mmmgo-11, p25
12	MgCl2 20M12 (1:10000)	19.6649	5.55	7/21/2008	Wipp-mmmgo-11, p25
13	MgCl2 20M13 (1:10000)	21.2213	5.99	7/3/2008	Wipp-mmmgo-11, p19
14	MgCl2 20M14 (1:10000)	21.7542	6.14	7/3/2008	Wipp-mmmgo-11, p19
15	MgCl2 20M15 (1:10000)	16.2091	4.57	7/22/2008	Wipp-mmmgo-11, p26
16	MgCl2 20M16 (1:10000)	17.2212	4.86	7/22/2008	Wipp-mmmgo-11, p26
17	MgCl2 20M17 (1:10000)	20.9420	5.91		
18	MgCl2 20M18 (1:10000)	20.1984	5.70		
19	MgCl2 20M19 (1:10000)	18.8557	5.32	8/4/2008	Wipp-mmmgo-11, p31
20	MgCl2 20M20 (1:10000)	18.4407	5.20	8/4/2008	Wipp-mmmgo-11, p31

MgCl2 20M18 (1:10000)	21.4076	6.04	7/7/2008	Wipp-mmmgo-11, p20
MgCl2 20M18 (1:10000)	18.9892	5.36	7/31/2008	Wipp-mmmgo-11, p30
MgCl2 20M17 (1:10000)	23.2622	6.56	7/7/2008	Wipp-mmmgo-11, p20
MgCl2 20M17 (1:10000)	18.6218	5.25	7/31/2008	Wipp-mmmgo-11, p30

1					
2					
3	MgCl23M3 (1:10000)	19.7374	5.57	7/1/2008	Wipp-mmmgo-11, p15
4					
5					
6					
7	MgCl2 3M7 (1:10000)	18.4638	5.21	7/17/2008	Wipp-mmmgo-11, p24
8	MgCl2 3M8 (1:10000)	18.2779	5.16	7/17/2008	Wipp-mmmgo-11, p24
9					
10					
11	MgCl2 3M11 (1:10000)	18.6266	5.25	7/17/2008	Wipp-mmmgo-11, p24
12	MgCl2 3M12 (1:10000)	19.3200	5.45	7/17/2008	Wipp-mmmgo-11, p24
13	MgCl2 3M13 (1:10000)	34.6706	9.78	7/3/2008	Wipp-mmmgo-11, p19
14	MgCl2 3M14 (1:10000)	20.8014	5.87	7/3/2008	Wipp-mmmgo-11, p19
15	MgCl2 3M15 (1:10000)	19.3756	5.47	7/23/2008	Wipp-mmmgo-11, p27
16	MgCl2 3M16 (1:10000)	18.9197	5.34	7/23/2008	Wipp-mmmgo-11, p27
17	MgCl2 3M17 (1:10000)	19.4004	5.47		
18	MgCl2 3M18 (1:10000)	19.2366	5.43		
19	MgCl2 3M19 (1:10000)	19.1148	5.39	8/4/2008	Wipp-mmmgo-11, p31
20	MgCl2 3M20 (1:10000)	19.1565	5.40	8/4/2008	Wipp-mmmgo-11, p31
21	MgCl23M21 (1:10000)	19.5893	5.53	6/23/2008	Wipp-mmmgo-11, p15
22	MgCl23M22 (1:10000)	19.7995	5.58	6/23/2008	Wipp-mmmgo-11, p15

MgCl2 3M4 (1:10000)	20.6373	5.82	7/9/2008	Wipp-mmmgo-11, p21
MgCl2 3M17 (1:10000)	20.8314	5.88	7/7/2008	Wipp-mmmgo-11, p20
MgCl2 3M17 (1:10000)	17.9694	5.07	7/31/2008	Wipp-mmmgo-11, p30
MgCl2 3M18 (1:10000)	20.2656	5.72	7/7/2008	Wipp-mmmgo-11, p20
MgCl2 3M18 (1:10000)	18.2075	5.14	7/31/2008	Wipp-mmmgo-11, p30

1					
2					
3	MgCl2 3S3 (1:10000)	20.0480	5.65	7/9/2008	Wipp-mmmgo-11, p21
4					
5	MgCl2 3S5 (1:10000)	20.3565	5.74	7/9/2008	Wipp-mmmgo-11, p21
6					
7	MgCl2 3S7 (1:10000)	18.8742	5.32	7/17/2008	Wipp-mmmgo-11, p24
8	MgCl2 3S8 (1:10000)	18.3363	5.17	7/17/2008	Wipp-mmmgo-11, p24
9					
10					
11	MgCl2 3S11 (1:10000)	18.4526	5.20	7/21/2008	Wipp-mmmgo-11, p25
12	MgCl2 3S12 (1:10000)	18.3819	5.18	7/21/2008	Wipp-mmmgo-11, p25
13	MgCl2 3S13 (1:10000)	20.0402	5.65	7/3/2008	Wipp-mmmgo-11, p19
14	MgCl2 3S14 (1:10000)	20.6127	5.81	7/3/2008	Wipp-mmmgo-11, p19
15	MgCl2 3S15 (1:10000)	19.5346	5.51	7/23/2008	Wipp-mmmgo-11, p27
16	MgCl2 3S16 (1:10000)	18.5184	5.22	7/23/2008	Wipp-mmmgo-11, p27
17	MgCl2 3S17 (1:10000)	19.6269	5.54		
18	MgCl2 3S18 (1:10000)	19.9958	5.64		
19	MgCl2 3S19 (1:10000)	18.9998	5.36	8/4/2008	Wipp-mmmgo-11, p31
20	MgCl2 3S20 (1:10000)	19.1313	5.40	8/4/2008	Wipp-mmmgo-11, p31
21	MgCl23S21 (1:10000)	19.4314	5.48	6/23/2008	Wipp-mmmgo-11, p15
22	MgCl23S22 (1:10000)	18.4048	5.19	6/23/2008	Wipp-mmmgo-11, p15

MgCl2 3S17 (1:10000)	20.4628	5.77	7/7/2008	Wipp-mmmgo-11, p20
MgCl2 3S17 (1:10000)	18.7911	5.30	7/31/2008	Wipp-mmmgo-11, p30
MgCl2 3S18 (1:10000)	20.9193	5.90	7/7/2008	Wipp-mmmgo-11, p20
MgCl2 3S18 (1:10000)	19.0723	5.38	7/31/2008	Wipp-mmmgo-11, p30

Raw Data: The scientific notebook and page number reference for the sample dilutions are given in column F
The measured Cl- concentrations in ppm, from ion-chromatography, are recorded in supplemental binder "MMMgO-Cl electrode-1".
The raw Cl- data can be found in the supplemental binder under the tab corresponding to the date of analysis listed in column E

Calculations: In column D, the Cl- concentration in mol/l is calculated by =
Cl concentration in column C / 10^3(conversion from ppm to g/L) / 35.4527 (molecular weight of Cl) x10000 (dilution factor)
Note: when the Cl- concentration in column C has been analyzed more than once, the average value is used.
For example, the result for sample MgCl2 3S17 (1:100000), given in cell C294, is the average of cells C312 and C313

Final result: The Cl- concentrations from column D are input into the Excel file "plots(review)", on the worksheet "raw data", on columns H, R, AD, AP, BB, BQ

			ICP-AES INFORMATION										
		ICP-AES Date	ICP-AES Raw	ICP-AES Raw		Procedure	Procedure	Dilution Information				Termination	
Sample ID			Conc. Mg (mg/l)	Conc. Ca (mg/l)	Dilution Factor	Mg Molarity (mol/l)	Ca Molarity (mol/l)	Notebook	Page	Notebook	Page	Notebook	Page
(MgCl2)20L	1	4/22/2008		2.704	66.67	0.0000	0.0045	10	46			5	75
(MgCl2)20L	2	4/22/2008		3.952	66.67	0.0000	0.0066	10	46			5	75
(MgCl2)20L	3	7/15/2008		56.2	3.33	0.0000	0.0047					5	79
(MgCl2)20L	3	7/16/2008	31.8		666.00	0.8714	0.0000					5	79
(MgCl2)20L	4	7/15/2008		53.7	3.33	0.0000	0.0045					5	79
(MgCl2)20L	4	7/16/2008	31.9		666.00	0.8741	0.0000					5	79
(MgCl2)20L	5	4/13/2007		54.7	3.33	0.0000	0.0045	6	77	5	84	6	11
(MgCl2)20L	5	6/28/2007	28.0		666.67	0.7680	0.0000	6	77	5	84	6	11
(MgCl2)20L	6	4/13/2007		55.2	3.33	0.0000	0.0046	6	77	5	84	6	11
(MgCl2)20L	6	6/28/2007	24.7		666.67	0.6775	0.0000	6	77	5	84	6	11
(MgCl2)20L	7	4/22/2008		3.309	66.67	0.0000	0.0055	10	46			6	28
(MgCl2)20L	8	4/22/2008		2.984	66.67	0.0000	0.0050	10	46			6	28
(MgCl2)20L	9	4/22/2008		1.034	200.00	0.0000	0.0052	10	46			6	29
(MgCl2)20L	10	4/22/2008		1.053	200.00	0.0000	0.0053	10	46			6	29
(MgCl2)20L	11	4/22/2008		1.079	200.00	0.0000	0.0054	10	46			6	50
(MgCl2)20L	12	4/22/2008		1.062	200.00	0.0000	0.0053	10	46			6	50
(MgCl2)20L	13	1/24/2008	19.7		Procedure	0.9321	0.0000					5	98
(MgCl2)20L	13	1/30/2008		5.89	Procedure	0.0000	0.0169					5	98
(MgCl2)20L	14	1/24/2008	18.7		Procedure	0.8848	0.0000					5	98
(MgCl2)20L	14	1/30/2008		5.96	Procedure	0.0000	0.0171					5	98
(MgCl2)20L	15	9/5/2007	26.2		Procedure	1.2397	0.0000					6	84
(MgCl2)20L	15	9/5/2007		2.08	Procedure	0.0000	0.0060					6	84
(MgCl2)20L	16	9/5/2007		2.21	Procedure	0.0000	0.0063					6	84
(MgCl2)20L	16	9/5/2007	24.5		Procedure	1.1592	0.0000					6	84
(MgCl2)20L	17	1/28/2008	23.7		Procedure	1.1214	0.0000					9	28
(MgCl2)20L	17	1/31/2008		2.082	Procedure	0.0000	0.0060					9	28
(MgCl2)20L	18	1/28/2008	23.7		Procedure	1.1214	0.0000					9	28
(MgCl2)20L	18	1/31/2008		1.839	Procedure	0.0000	0.0053					9	28
(MgCl2)20L	19	4/21/2008	24.3		Procedure	1.1498	0.0000	10	44			10	44
(MgCl2)20L	19	4/22/2008		2.165	Procedure	0.0000	0.0062	10	44			10	44
(MgCl2)20L	20	4/21/2008	24		Procedure	1.1356	0.0000	10	44			10	44
(MgCl2)20L	20	4/22/2008		2.028	Procedure	0.0000	0.0058	10	44			10	44

Sample ID		ICP-AES Date	ICP-AES Raw Conc. Mg (mg/l)	ICP-AES Raw Conc. Ca (mg/l)	Dilution Factor	Procedure Mg Molarity (mol/l)	Procedure Ca Molarity (mol/l)	Dilution Information Notebook	Page	Notebook	Page	Termination Notebook	Page
(MgCl2)20M	1	4/22/2008		2.95	66.67	0.0000	0.0049	10	46			5	75
(MgCl2)20M	2	4/22/2008		2.73	66.67	0.0000	0.0045	10	46			5	75
(MgCl2)20M	3	7/15/2008		57.1	3.33	0.0000	0.0047					5	79
(MgCl2)20M	3	7/16/2008	30.1		666.00	0.8248	0.0000					5	79
(MgCl2)20M	4	7/15/2008		58.2	3.33	0.0000	0.0048					5	79
(MgCl2)20M	4	7/16/2008	31.2		666.00	0.8549	0.0000					5	79
(MgCl2)20M	5	4/13/2007		58.2	3.33	0.0000	0.0048	6	77	5	84	6	11
(MgCl2)20M	5	6/28/2007	24.2		666.67	0.6638	0.0000	6	77	5	84	6	11
(MgCl2)20M	6	4/13/2007		58.6	3.33	0.0000	0.0049	6	77	5	84	6	11
(MgCl2)20M	6	No Mg Test				#VALUE!	#VALUE!	6	77	5	84	6	11
(MgCl2)20M	7	4/22/2008		3.211	66.67	0.0000	0.0053	10	46			6	28
(MgCl2)20M	8	4/22/2008		3.342	66.67	0.0000	0.0056	10	46			6	28
(MgCl2)20M	9	4/22/2008		1.055	200.00	0.0000	0.0053	10	46			6	29
(MgCl2)20M	10	4/22/2008		1.178	200.00	0.0000	0.0059	10	46			6	29
(MgCl2)20M	11	4/22/2008		1.05	200.00	0.0000	0.0052	10	46			6	50
(MgCl2)20M	12	4/22/2008		1.011	200.00	0.0000	0.0050	10	46			6	50
(MgCl2)20M	13	1/24/2008	19.1		Procedure	0.9037	0.0000					5	98
(MgCl2)20M	13	1/30/2008		5.81	Procedure	0.0000	0.0167					5	98
(MgCl2)20M	14	1/24/2008	16.4		Procedure	0.7760	0.0000					5	98
(MgCl2)20M	14	1/30/2008		5.9	Procedure	0.0000	0.0169					5	98
(MgCl2)20M	15	9/5/2007	20.2		Procedure	0.9558	0.0000					6	84
(MgCl2)20M	15	9/5/2007		1.91	Procedure	0.0000	0.0055					6	84
(MgCl2)20M	16	9/5/2007	21.8		Procedure	1.0315	0.0000					6	84
(MgCl2)20M	16	9/5/2007		1.97	Procedure	0.0000	0.0057					6	84
(MgCl2)20M	17	1/28/2008	23.3		Procedure	1.1024	0.0000					9	28
(MgCl2)20M	17	1/31/2008		2.264	Procedure	0.0000	0.0065					9	28
(MgCl2)20M	18	1/28/2008	23		Procedure	1.0883	0.0000					9	28
(MgCl2)20M	18	1/31/2008		17.56	Procedure	0.0000	0.0504					9	28
(MgCl2)20M	19	4/21/2008	23		Procedure	1.0883	0.0000	10	44			10	44
(MgCl2)20M	19	4/22/2008		2.204	Procedure	0.0000	0.0063	10	44			10	44
(MgCl2)20M	20	4/21/2008	22.8		Procedure	1.0788	0.0000	10	44			10	44
(MgCl2)20M	20	4/22/2008		2.144	Procedure	0.0000	0.0062	10	44			10	44

		ICP-AES Date	ICP-AES Raw	ICP-AES Raw		Procedure	Procedure	Dilution Information				Termination	
Sample ID			Conc. Mg (mg/l)	Conc. Ca (mg/l)	Dilution Factor	Mg Molarity (mol/l)	Ca Molarity (mol/l)	Notebook	Page	Notebook	Page	Notebook	Page
(MgCl2)3M	1	4/23/2008		19.1	66.67	0.0000	0.0318	10	46			5	75
(MgCl2)3M	2	4/23/2008		19.1	66.67	0.0000	0.0318	10	46			5	75
(MgCl2)3M	3	6/27/2007		19.3	66.67	0.0000	0.0321	6	77	5	84	5	79
(MgCl2)3M	3	6/28/2007	26.0		666.67	0.7132	0.0000	6	77	5	84	5	79
(MgCl2)3M	4	6/27/2007		19.1	66.67	0.0000	0.0318	6	77	5	84	5	79
(MgCl2)3M	4	6/28/2007	27.1		666.67	0.7433	0.0000	6	77	5	84	5	79
(MgCl2)3M	5	6/27/2007		42.0	33.33	0.0000	0.0349	6	77	5	84	6	11
(MgCl2)3M	5	6/28/2007	38.2		333.33	0.5239	0.0000	6	77	5	84	6	11
(MgCl2)3M	6	6/27/2007		40.6	33.33	0.0000	0.0338	6	77	5	84	6	11
(MgCl2)3M	6	6/28/2007	36.5		333.33	0.5006	0.0000	6	77	5	84	6	11
(MgCl2)3M	7	4/23/2008		24.6	66.67	0.0000	0.0409	10	46			6	28
(MgCl2)3M	8	4/23/2008		25.3	66.67	0.0000	0.0421	10	46			6	28
(MgCl2)3M	9	4/23/2008	84.4	9.51	200.00	0.6945	0.0475	10	46			6	29
(MgCl2)3M	10	4/23/2008	77	8.56	200.00	0.6336	0.0427	10	46			6	29
(MgCl2)3M	11	4/23/2008	79.5	9.51	200.00	0.6542	0.0475	10	46			6	50
(MgCl2)3M	12	4/23/2008	83.5	10.1	200.00	0.6871	0.0504	10	46			6	50
(MgCl2)3M	13	1/24/2008	14.2		Procedure	0.6719	0.0000					5	98
(MgCl2)3M	13	1/30/2008		21	Procedure	0.0000	0.0603					5	98
(MgCl2)3M	14	1/24/2008	14		Procedure	0.6624	0.0000					5	98
(MgCl2)3M	14	1/30/2008		22.3	Procedure	0.0000	0.0640					5	98
(MgCl2)3M	15	9/5/2007	17.9		Procedure	0.8469	0.0000					6	84
(MgCl2)3M	15	9/5/2007		17.5	Procedure	0.0000	0.0502					6	84
(MgCl2)3M	16	9/5/2007	18.2		Procedure	0.8611	0.0000					6	84
(MgCl2)3M	16	9/5/2007		18.6	Procedure	0.0000	0.0534					6	84
(MgCl2)3M	17	1/28/2008	17.9		Procedure	0.8469	0.0000					9	28
(MgCl2)3M	17	1/31/2008		17.16	Procedure	0.0000	0.0492					9	28
(MgCl2)3M	18	1/28/2008	17.4		Procedure	0.8233	0.0000					9	28
(MgCl2)3M	18	1/31/2008		16.8	Procedure	0.0000	0.0482					9	28
(MgCl2)3M	19	4/21/2008	19.3	0	Procedure	0.9132	0.0000	10	44			10	44
(MgCl2)3M	19	4/22/2008		17.61	Procedure	0.0000	0.0505	10	44			10	44
(MgCl2)3M	20	4/21/2008	18		Procedure	0.8517	0.0000	10	44			10	44
(MgCl2)3M	20	4/22/2008		17.47	Procedure	0.0000	0.0501	10	44			10	44
(MgCl2)3M	21	7/15/2008	14.5	21.8	Procedure	0.6861	0.0626					9	87
(MgCl2)3M	22	7/15/2008	13.6	20.6	Procedure	0.6435	0.0591					9	87

		ICP-AES Date	ICP-AES Raw	ICP-AES Raw		Procedure	Procedure	Dilution Information				Termination	
Sample ID			Conc. Mg (mg/l)	Conc. Ca (mg/l)	Dilution Factor	Mg Molarity (mol/l)	Ca Molarity (mol/l)	Notebook	Page	Notebook	Page	Notebook	Page
(MgCl2)3s	1	4/22/2008		18.47	66.67	0.0000	0.0307	10	46			5	75
(MgCl2)3s	2	4/22/2008		18.99	66.67	0.0000	0.0316	10	46			5	75
(MgCl2)3S	3	6/27/2007		20.5	66.67	0.0000	0.0341	6	77	5	84	5	79
(MgCl2)3S	3	6/28/2007	11.9		666.67	0.3264	0.0000	6	77	5	84	5	79
(MgCl2)3S	4	6/27/2007		20.6	66.67	0.0000	0.0343	6	77	5	84	5	79
(MgCl2)3S	4	6/28/2007	21.7		666.67	0.5952	0.0000	6	77	5	84	5	79
(MgCl2)3S	5	6/27/2007		42.1	33.33	0.0000	0.0350	6	77	5	84	6	11
(MgCl2)3S	5	6/28/2007	33.3		333.33	0.4567	0.0000	6	77	5	84	6	11
(MgCl2)3S	6	6/27/2007		43.3	33.33	0.0000	0.0360	6	77	5	84	6	11
(MgCl2)3S	6	6/28/2007	26.3		333.33	0.3607	0.0000	6	77	5	84	6	11
(MgCl2)3s	7	4/22/2008		23.71	66.67	0.0000	0.0394	10	46			6	28
(MgCl2)3s	8	4/22/2008		24.37	66.67	0.0000	0.0405	10	46			6	28
(MgCl2)3s	9	4/22/2008		8.679	200.00	0.0000	0.0433	10	46			6	29
(MgCl2)3s	10	4/22/2008		10.03	200.00	0.0000	0.0501	10	46			6	29
(MgCl2)3s	11	4/22/2008		9.121	200.00	0.0000	0.0455	10	46			6	50
(MgCl2)3s	12	4/22/2008		9.422	200.00	0.0000	0.0470	10	46			6	50
(MgCl2)3s	13	1/24/2008	12		Procedure	0.5678	0.0000					5	98
(MgCl2)3s	13	1/30/2008		23.1	Procedure	0.0000	0.0663					5	98
(MgCl2)3s	14	1/24/2008	12.4		Procedure	0.5867	0.0000					5	98
(MgCl2)3s	14	1/30/2008		22.3	Procedure	0.0000	0.0640					5	98
(MgCl2)3s	15	9/5/2007	16		Procedure	0.7570	0.0000					6	84
(MgCl2)3s	15	9/5/2007		18.8	Procedure	0.0000	0.0539					6	84
(MgCl2)3s	16	9/5/2008	15.9		Procedure	0.7523	0.0000					6	84
(MgCl2)3s	16	9/5/2008		18.5	Procedure	0.0000	0.0531					6	84
(MgCl2)3s	17	1/28/2008	15.8		Procedure	0.7476	0.0000					9	28
(MgCl2)3s	17	1/31/2008		17.48	Procedure	0.0000	0.0502					9	28
(MgCl2)3s	18	1/28/2008	16.6		Procedure	0.7854	0.0000					9	28
(MgCl2)3s	18	1/31/2008		1.986	Procedure	0.0000	0.0057					9	28
(MgCl2)3s	19	4/21/2008	18.1		Procedure	0.8564	0.0000	10	44			10	44
(MgCl2)3s	19	4/22/2008		17.89	Procedure	0.0000	0.0513	10	44			10	44
(MgCl2)3s	20	4/21/2008	17.1		Procedure	0.8091	0.0000	10	44			10	44
(MgCl2)3s	20	4/22/2008		16.49	Procedure	0.0000	0.0473	10	44			10	44
(MgCl2)3s	21	7/15/2008	15		Procedure	0.7097	0.0000	9	89			9	87
(MgCl2)3s	21	7/15/2008		20.8	Procedure	0.0000	0.0597	9	89			9	87
(MgCl2)3s	22	7/15/2008	14.9		Procedure	0.7050	0.0000	9	89			9	87
(MgCl2)3s	22	7/15/2008		20	Procedure	0.0000	0.0574	9	89			9	87

		ICP-AES Date	ICP-AES Raw	ICP-AES Raw		Procedure	Procedure	Dilution Information				Termination	
Sample ID			Conc. Mg (mg/l)	Conc. Ca (mg/l)	Dilution Factor	Mg Molarity (mol/l)	Ca Molarity (mol/l)	Notebook	Page	Notebook	Page	Notebook	Page
ER20M	1	4/23/2008	7.56	7.85	66.67	0.0207	0.0131	10	46			5	75
ER20M	2	4/23/2008	7.46	7.52	66.67	0.0205	0.0125	10	46			5	75
ER20M	3					0.0000	0.0000					5	79
ER20M	4					0.0000	0.0000					5	79
ER20M	5	4/23/2008	3.67	9.63	66.67	0.0101	0.0160	10	46			6	28
ER20M	6	4/23/2008	6.29	9.78	66.67	0.0173	0.0163	10	46			6	28
ER20M	7	4/23/2008	0.847	2.82	200.00	0.0070	0.0141	10	46			6	50
ER20M	8	4/23/2008	1.01	3.34	200.00	0.0083	0.0167	10	46			6	50
ER20M	9	9/5/2007	0.339		Procedure	0.0160	0.0000					6	84
ER20M	9	9/5/2007		5.21	Procedure	0.0000	0.0149					6	84
ER20M	10	9/5/2007		5.27	Procedure	0.0000	0.0151					6	84
ER20M	10	9/5/2007	0.265		Procedure	0.0125	0.0000					6	84
ER20M	11	1/31/2008		5.43	115.00	0.0000	0.0156					10	9
ER20M	12	1/31/2008		4.882	115.00	0.0000	0.0140					10	9
ER20M	13	7/15/2008	1.4	6.54	115.00	0.0066	0.0188					9	87
ER20M	14	7/15/2008	1.44	6.29	115.00	0.0068	0.0180					9	87
ER20s	1	4/23/2008	16.7	20	33.33	0.0229	0.0166	10	46			5	75
ER20s	2	4/23/2008	15.7	13.6	33.33	0.0215	0.0113	10	46			5	75
ER20s	3					0.0000	0.0000					5	79
ER20s	4					0.0000	0.0000					5	79
ER20S	5	6/27/2007		50.1	6.66	0.0000	0.0083			5	84	6	11
ER20S	5	6/27/2007	53.2		6.66	0.0146	0.0000			5	84	6	11
ER20S	6	6/27/2007		47.3	6.66	0.0000	0.0079			5	84	6	11
ER20S	6	6/27/2007	49.9		6.66	0.0137	0.0000			5	84	6	11
ER20s	7	4/23/2008	12.8	13.5	33.33	0.0176	0.0112	10	46			6	28
ER20s	8	4/23/2008	11.7	13.5	33.33	0.0160	0.0112	10	46			6	28
ER20s	9					#VALUE!	#VALUE!					6	29
ER20s	10					#VALUE!	#VALUE!					6	29
ER20s	11					#VALUE!	#VALUE!					6	50
ER20s	12					#VALUE!	#VALUE!					6	50
ER20s	13	9/5/2007	2.09	4.1	Procedure	0.0989	0.0118					6	84
ER20s	14	9/5/2007	1.78	4.46	Procedure	0.0842	0.0128					6	84
ER20s	15	1/31/2008		4.269	Procedure	0.0000	0.0122					10	9
ER20s	16	1/31/2008		4.221	Procedure	0.0000	0.0121					10	9
ER20s	17	7/15/2008	2.47	5.07	115.00	0.0117	0.0145					9	87
ER20s	18	7/15/2008	2.71	5.29	115.00	0.0128	0.0152					9	87

		ICP-AES Date	ICP-AES Raw	ICP-AES Raw		Procedure	Procedure	Dilution Information				Termination	
Sample ID			Conc. Mg (mg/l)	Conc. Ca (mg/l)	Dilution Factor	Mg Molarity (mol/l)	Ca Molarity (mol/l)	Notebook	Page	Notebook	Page	Notebook	Page
ER3L	1	4/23/2008	58.3	25.8	33.33	0.0800	0.0215	10	46			5	75
ER3L	2	4/23/2008	14.4	25	33.33	0.0197	0.0208	10	46			5	75
ER3L	3	6/27/2007	2.11		33.33	0.0029	0.0000			5	84	5	79
ER3L	3	6/27/2007		23.7	33.33	0.0000	0.0197			5	84	5	79
ER3L	4	6/27/2007	2.05		33.33	0.0028	0.0000			5	84	5	79
ER3L	4	6/27/2007		23.5	33.33	0.0000	0.0195			5	84	5	79
ER3L	5	4/23/2008	0.013	22.2	33.33	0.0000	0.0185	10	46			6	28
ER3L	6	4/23/2008	-0.011	23.3	33.33	0.0000	0.0194	10	46			6	28
ER3L	7	4/23/2008	-0.195	67.3	100.00	-0.0008	0.1679	10	46			6	50
ER3L	8	4/23/2008	-0.171	61.3	100.00	-0.0007	0.1530	10	46			6	50
ER3L	9	4/23/2008	40.1	49.1	115.00	0.1897	0.1409	6	84			6	84
ER3L	10	4/23/2008	39.2	48.7	115.00	0.1855	0.1397	6	84			6	84
ER3M	1	4/23/2008	10.7	19.2	33.33	0.0147	0.0160	10	46			5	75
ER3M	2	4/23/2008	10.1	19.8	33.33	0.0139	0.0165	10	46			5	75
ER3M	3	4/13/2007	55.1		3.33	0.0076	0.0000					5	79
ER3M	3	6/27/2007		36.9	16.67	0.0000	0.0153			5	84	5	79
ER3M	4	4/13/2007	43.5		3.33	0.0060	0.0000					5	79
ER3M	4	6/27/2007		36.8	16.67	0.0000	0.0153			5	84	5	79
ER3M	5	4/23/2008	-0.224	20.4	33.33	-0.0003	0.0170	10	46			6	28
ER3M	6	4/23/2008		21.2	33.33	0.0000	0.0176	10	46			6	28
ER3M	7	4/23/2008	-0.114	65.3	10.00	0.0000	0.0163	6	50			6	50
ER3M	8	4/23/2008	-0.167	65.9	10.00	-0.0001	0.0164	6	50			6	50
ER3M	9	2/21/2008		7.321	115.00	0.0000	0.0210	6	50			6	50
ER3M	10	2/21/2008		3.165	115.00	0.0000	0.0091	6	50			6	50

		ICP-AES Date	ICP-AES Raw	ICP-AES Raw		Procedure	Procedure	Dilution Information				Termination	
Sample ID			Conc. Mg (mg/l)	Conc. Ca (mg/l)	Dilution Factor	Mg Molarity (mol/l)	Ca Molarity (mol/l)	Notebook	Page	Notebook	Page	Notebook	Page
GW20L	1	4/22/2008		7.758	66.67	0.0000	0.0129	10	46			5	75
GW20L	2	4/22/2008		7.907	66.67	0.0000	0.0132	10	46			5	75
GW20L	3					0.0000	0.0000					5	79
GW20L	4					0.0000	0.0000					5	79
GW20L	5	4/22/2008		8.323	66.67	0.0000	0.0138	10	46			6	28
GW20L	5	4/23/2008		8.378	66.67	0.0000	0.0139	10	46			6	28
GW20L	6	4/23/2008		8.217	66.67	0.0000	0.0137	10	46			6	28
GW20L	6	4/22/2008		8.269	66.67	0.0000	0.0138	10	46			6	28
GW20L	7	4/22/2008		3.224	200.00	0.0000	0.0161	10	46			6	50
GW20L	7	4/23/2008		3.168	200.00	0.0000	0.0158	10	46			6	50
GW20L	8	4/22/2008		3.428	200.00	0.0000	0.0171	10	46			6	50
GW20L	9	9/5/2007	25.3		Procedure	1.1971	0.0000					6	84
GW20L	9	9/5/2007		5.68	Procedure	0.0000	0.0163					6	84
GW20L	10	9/5/2007		5.87	Procedure	0.0000	0.0168					6	84
GW20L	10	9/5/2007	25.4		Procedure	1.2018	0.0000					6	84
GW20L	11	2/21/2008	21.7		Procedure	1.0267	#VALUE!					10	11
GW20L	11	2/21/2008		8.345	Procedure	0.0000	0.0239					10	11
GW20L	12	2/21/2008	23.9		Procedure	1.1308	0.0000					10	11
GW20L	12	2/21/2008		8.612	Procedure	#VALUE!	0.0247					10	11
GW20M	1	4/22/2008		7.099	66.67	0.0000	0.0118	10	46			5	75
GW20M	2	4/22/2008		7.907	66.67	0.0000	0.0132	10	46			5	75
GW20M	3	6/27/2007		13.3	33.33	0.0000	0.0111	6	77	5	84	5	79
GW20M	3	6/28/2007	62.5		333.33	0.8572	0.0000	6	77	5	84	5	79
GW20M	4	6/27/2007		12.8	33.33	0.0000	0.0106	6	77	5	84	5	79
GW20M	4	6/28/2007	59.5		333.33	0.8160	0.0000	6	77	5	84	5	79
GW20M	5	4/22/2008		8.275	66.67	0.0000	0.0138	10	46			6	28
GW20M	5	4/22/2008		8.208	66.67	0.0000	0.0137	10	46			6	28
GW20M	6	4/22/2008		8.046	66.67	0.0000	0.0134	10	46			6	28
GW20M	6	4/22/2008		8.222	66.67	0.0000	0.0137	10	46			6	28
GW20M	7	4/22/2008		3.083	200.00	0.0000	0.0154	10	46			6	50
GW20M	7	4/22/2008		3.074	200.00	0.0000	0.0153	10	46			6	50
GW20M	8	4/22/2008		2.834	200.00	0.0000	0.0141	10	46			6	50
GW20M	9	9/5/2007		5.87	Procedure	0.0000	0.0168					6	84
GW20M	9	9/5/2007	23.6		Procedure	1.1166	0.0000					6	84
GW20M	10	9/5/2007		6.02	Procedure	0.0000	0.0173					6	84
GW20M	10	9/5/2007	23.8		Procedure	1.1261	0.0000					6	84
GW20M	11	2/21/2008	22.6		Procedure	1.0693	0.0000					10	9
GW20M	11	2/21/2008		8.718	Procedure	0.0000	0.0250					10	9
GW20M	12	2/21/2008	21.8		Procedure	1.0315	0.0000					10	9
GW20M	12	2/21/2008		8.328	Procedure	0.0000	0.0239					10	9

		ICP-AES Date	ICP-AES Raw	ICP-AES Raw		Procedure	Procedure	Dilution Information				Termination		
Sample ID			Conc. Mg (mg/l)	Conc. Ca (mg/l)	Dilution Factor	Mg Molarity (mol/l)	Ca Molarity (mol/l)	Notebook	Page	Notebook	Page	Notebook	Page	
GW3M	1	4/23/2008		17.2	33.33	0.0000	0.0143	10	46			5	75	
GW3M	1	4/23/2008	66		333.33	0.9052	#VALUE!	10	46			5	75	
GW3M	2	4/23/2008		17.8	33.33	0.0000	0.0148	10	46			5	75	
GW3M	2	4/23/2008	64.6		333.33	0.8860	#VALUE!	10	46			5	75	
GW3M	3	6/27/2007		36.7	166.67	0.0000	0.1526	6	77	5	84	5	79	
GW3M	3	6/28/2007	11.5		1666.67	0.7886	0.0000	6	77	5	84	5	79	
GW3M	4	6/27/2007		44.4	166.67	0.0000	0.1846	6	77	5	84	5	79	
GW3M	4	6/28/2007			1666.67	0.0000	0.0000	6	77	5	84	5	79	
GW3M	5	4/23/2008	61.1		333.33	0.8380	#VALUE!	10	46			6	28	
GW3M	5	4/23/2008		18.3	33.33	0.0000	0.0152	10	46			6	28	
GW3M	6	4/23/2008		16.8	33.33	0.0000	0.0140	10	46			6	28	
GW3M	6	4/23/2008	57		333.33	0.7817	#VALUE!	10	46			6	28	
GW3M	7	4/23/2008		7.25	100.00	0.0000	0.0181	10	46			6	50	
GW3M	7	4/23/2008	18.5		1000.00	0.7612	#VALUE!	10	46			6	50	
GW3M	8	4/23/2008	16.9		1000.00	0.6953	0.0000	10	46			6	50	
GW3M	8	4/23/2008		6.51	100.00	0.0000	0.0162	10	46					
GW3M	9	9/5/2007		5.93	Procedure	0.0000	0.0170					6	84	
GW3M	9	9/5/2007	16.4		Procedure	0.7760	0.0000					6	84	
GW3M	10	9/5/2007	16.4		Procedure	0.7760	0.0000					6	84	
GW3M	10	9/5/2007		5.99	Procedure	0.0000	0.0172					6	84	
GW3M	11	1/28/2008	16.2		Procedure	0.7665	0.0000					10	9	
GW3M	11	1/31/2008		5.301	Procedure	0.0000	0.0152					10	9	
GW3M	12	1/28/2008	16		Procedure	0.7570	0.0000					10	9	
GW3M	12	1/31/2008		5.443	Procedure	0.0000	0.0156					10	9	
GW3M	13	7/15/2008	12.5	6.49	Procedure	0.5914	0.0186					9	87	
GW3M	14	7/15/2008	14.4	7.52	Procedure	0.6813	0.0216					9	87	

		ICP-AES Date	ICP-AES Raw	ICP-AES Raw		Procedure	Procedure	Dilution Information				Termination	
Sample ID			Conc. Mg (mg/l)	Conc. Ca (mg/l)	Dilution Factor	Mg Molarity (mol/l)	Ca Molarity (mol/l)	Notebook	Page	Notebook	Page	Notebook	Page
GW3S	1	4/22/2008		11.86	66.67	0.0000	0.0197	10	46			5	75
GW3S	2				66.67	0.0000	0.0000	10	46			5	75
GW3S	3	6/27/2007		10.6	66.67	0.0000	0.0176	6	77	5	84	5	79
GW3S	3	6/28/2007	26.4		666.67	0.7241	0.0000	6	77	5	84	5	79
GW3S	4	6/27/2007		10.1	66.67	0.0000	0.0168	6	77	5	84	5	79
GW3S	4	6/28/2007	24.5		666.67	0.6720	0.0000	6	77	5	84	5	79
GW3S	5	6/27/2007		8.62	66.67	0.0000	0.0143	6	77	5	84	6	11
GW3S	5	6/28/2007	23.5		666.67	0.6446	0.0000	6	77	5	84	6	11
GW3S	6	6/27/2007		9.14	66.67	0.0000	0.0152	6	77	5	84	6	11
GW3S	6	6/28/2007	20.9		666.67	0.5733	0.0000	6	77	5	84	6	11
GW3S	7	4/22/2008		10.91	66.67	0.0000	0.0181	10	46			6	28
GW3S	7	4/22/2008		9.48	66.67	0.0000	0.0158	10	46			6	28
GW3S	8	4/22/2008		11.1	66.67	0.0000	0.0185	10	46			6	28
GW3S	8	4/23/2008		10.04	66.67	0.0000	0.0167	10	46			6	28
GW3S	9	4/22/2008		3.427	200.00	0.0000	0.0171	10	46			6	29
GW3S	9	4/23/2008		3.324	200.00	0.0000	0.0166	10	46			6	29
GW3S	10	4/23/2008	87.3	3.52	200.00	0.7184	0.0176	10	46			6	29
GW3S	11	4/23/2008	88.1	3.66	200.00	0.7250	0.0183	10	46			6	50
GW3S	12	4/23/2008	85.7	3.47	200.00	0.7052	0.0173	10	46			6	50
GW3S	13	9/5/2007	18.7		Procedure	0.8848	0.0000					6	84
GW3S	13	9/5/2007		6.08	Procedure	0.0000	0.0174					6	84
GW3S	14	9/5/2007	18.7		Procedure	0.8848	0.0000					6	84
GW3S	14	9/5/2007		5.97	Procedure	0.0000	0.0171					6	84
GW3S	15	1/28/2008	17.8		Procedure	0.8422	0.0000					9	28
GW3S	15	1/31/2008		5.205	Procedure	0.0000	0.0149					9	28
GW3S	16	1/28/2008	18.5		Procedure	0.8753	0.0000					9	28
GW3S	16	1/31/2008		5.262	Procedure	0.0000	0.0151					9	28
GW3S	17	7/15/2008	16.7	7.74	Procedure	0.7902	0.0222					9	87
GW3S	18	7/15/2005	13.8	6.5	Procedure	0.6530	0.0187					9	87

Raw Data: The ICP-AES analysis date in column C is recorded in the supplemental binder "MMMgO-ICP-AES-1".
The Mg concentration in ppm (mg/l) in column D can be found in supplemental binder "MMMgO-ICP-AES-1",
which is organized by the analysis date, which is given in column C.
The Ca concentration in ppm (mg/l) in column E can be found in supplemental binder "MMMgO-ICP-AES-1" in the same way as the Mg data.

The Dilution information is recorded in the scientific notebook ,see column I, J, K, L, and M, N
The notebook numbers in columns I and N correspond to WIPP-MM MgO-#
Termination information (sample collection date) is can be found in the scientific notebook ,see column M, N

Calculations: The dilution factor in column F can be found in the scientific notebooks ,see column I, J, K, L, M, N.
Column F can be a number or "procedure":
"Procedure" can be found in WIPP-MMMgO-6, P79.
If column F = procedure, then the sample hydrated in GWB or Simplified GWB has been diluted 1150 times for Mg analysis
If column F = procedure, then the sample hydrated in GWB or Simplified GWB has been diluted 115 times for Ca analysis
If column F = procedure, then the sample hydrated in ERDA-6 has been diluted 115 times for Ca analysis
If column F = procedure, then the sample hydrated in ERDA-6 has been diluted 1150 times for Mg analysis.
Note the dilution factor for the sample hydrated in ERDA-6 for Mg analysiswas was changed to 115 after 12/14/07.
To make the calculation simple, set the dilution factor to 115 for sample diluted after 12/14 /07 .
If column F is not = procedure, then the sample dilution factor is calculated from dilution process documented in the scientific notebook, see columns I, J, K, L, M, N.
For example, Cell F282 = 20x10 = 200. Sample GW3S12 was first diluted 10 times (documented on WIPP-MMMgO-6,p50), then diluted 20 times (WIPP-MMMgO-10, P46).

The Mg molarity (mol/l) in column G = Mg concentration in column D (mg/l) X dilution factor in column F/ 1000 (conversion from mg/l to g/l) / 24.305 (molecular weight of Mg)
The Ca molarity in column H = Ca concentration in column E (mg/l) X dilution factor in column F / 1000 (conversion from mg/l to g/l) / 40.078 (molecular weight of Ca)

Output: The Mg molarity (mol/l) in column G and Ca molarity in column H is inputted into the Excel file "plots(review)", on worksheet "raw data" , on columns S, T, AE, AF, BC, BD, BR, BS.

Reaction $HSO_4^- = H^+ + SO_4^{2-}$

Brine	H+ (M)	SO42- (M)	HSO4- (M)	H+ (m)	SO42- (m)	HSO4- (m)	log Ka, molar scale	log Ka, molal scale
GWB	3.34709E-09	1.68809E-01	5.14351E-09	3.81225E-09	1.92269E-01	5.85831E-09	-0.9592	-0.9027
ERDA-6	5.10858E-02	9.93138E-02	7.14942E-02	5.74481E-02	1.11682E-01	8.03982E-02	-1.1490	-1.0980

These values can be found in the FMT files: fmt_aciddis_2009_msrpt_GWB_001.OUT; fmt_aciddis_2009_msrpt_erda6_002.OUT, which are located in CMS in the class LIBACIDDIS_FMT

This worksheet is a summary of the slopes obtained from titrating ERDA-6, simplified GWB, and GWB with HCl
The slopes for each row below can be found on the corresponding worksheet, for example for row 5 see the worksheet titled "ERDA with HCl1"

ERDA-6

	slope	log(slope)	R2		
HCl 1	13.959	1.144854	0.9934	1.155	Avg of log(slope)
HCl 2	14.127	1.15005	0.9994	0.013	Standard deviation of log(slope)
HCl 3	14.785	1.169821	0.9997		

Simple GWB

	slope	log(slope)	R2		
HCl 1	15.587	1.192763	0.9924	1.206	Avg of log(slope)
HCl 2	15.481	1.189799	0.995	0.025	Standard deviation of log(slope)
HCl 3	17.169	1.234745	0.9926		

GWB

	slope	log(slope)	R2		
HCl 1	16.686	1.222352	0.9998	1.236	Avg of log(slope)
HCl 2	18.124	1.258254	0.9996	0.019	Standard deviation of log(slope)
HCl 3	16.896	1.227784	0.9995		

Brine: GWB   Temperature:25.02°C   Start Time: 5:00pm
Titrant 1.00M HCl   End Time: 6:05pm
Notebook and pg: Wipp-MMMgO-14 p.15

amt added mL	Total Added mL	pH observed	H+ Observed (M)	HCl added (M)	H+ free (M)
0	0	7.46	3.467E-08		
0.1	0.1	7.43	3.715E-08		
0.1	0.2	7.4	3.981E-08		
0.1	0.3	7.37	4.266E-08		
0.1	0.4	7.34	4.571E-08		
0.1	0.5	7.31	4.898E-08		
0.1	0.6	7.28	5.248E-08		
0.1	0.7	7.24	5.754E-08		
0.1	0.8	7.21	6.166E-08		
0.1	0.9	7.14	7.244E-08		
0.1	1	7.11	7.762E-08		
0.1	1.1	7.08	8.318E-08		
0.1	1.2	7.04	9.120E-08		
0.1	1.3	7.01	9.772E-08		
0.1	1.4	6.97	1.072E-07		
0.1	1.5	6.93	1.175E-07		
0.1	1.6	6.89	1.288E-07		
0.1	1.7	6.85	1.413E-07		
0.1	1.8	6.81	1.549E-07		
0.1	1.9	6.77	1.698E-07		
0.1	2	6.73	1.862E-07		
0.1	2.1	6.68	2.089E-07		
0.1	2.2	6.63	2.344E-07		
0.1	2.3	6.58	2.630E-07		
0.1	2.4	6.52	3.020E-07		
0.1	2.5	6.47	3.388E-07		
0.1	2.6	6.4	3.981E-07		
0.1	2.7	6.33	4.677E-07		
0.1	2.8	6.25	5.623E-07		
0.1	2.9	6.16	6.918E-07		
0.1	3	6.06	8.710E-07		
0.1	3.1	5.93	1.175E-06		
0.1	3.2	5.77	1.698E-06		
0.1	3.3	5.53	2.951E-06		
0.1	3.4	5.07	8.511E-06		
0.1	3.5	2.42	3.802E-03	0.000E+00	0.000E+00
0.05	3.55	2.03	9.333E-03	9.337E-04	3.563E-04
0.05	3.6	1.82	1.514E-02	1.866E-03	7.120E-04
0.05	3.65	1.68	2.089E-02	2.796E-03	1.067E-03
0.05	3.7	1.57	2.692E-02	3.724E-03	1.421E-03
0.05	3.75	1.49	3.236E-02	4.651E-03	1.775E-03
0.05	3.8	1.42	3.802E-02	5.576E-03	2.128E-03
0.05	3.85	1.35	4.467E-02	6.500E-03	2.480E-03
0.05	3.9	1.3	5.012E-02	7.421E-03	2.832E-03
0.1	4	1.21	6.166E-02	9.259E-03	3.534E-03
0.1	4.1	1.13	7.413E-02	1.109E-02	4.232E-03
0.1	4.2	1.07	8.511E-02	1.292E-02	4.929E-03
0.1	4.3	1.01	9.772E-02	1.473E-02	5.622E-03

1+ (1/Ka) x [SO42-] =   2.620E+00

Data location   Wipp-MMMgO-14 p.15
Calculation steps:

1 H+ Observed in column D = 10^-pH observed in column C
2 Plot pH observed (column C) against total acid added (column B), Figure 1, and determine the equivalence volume, 3.50 ml
3 H+ added in column E =
(Total added acid in column B - equivalence volume 3.50 ml) x HCl concentration/(Brine volume 50ml + Total volume of added acid in column B)
HCl concentration is given in notebook wipp-FePb-1, p6 and p21.
4 H+ free in column F = H+ added in column E/ value in cell I27 using equation (6) in section 3.3 of the report.
5 Here cell I27 =1+ (1/Ka)x [SO42-] with Ka =10^(-0.9592),
where Ka is given in worksheet "constant", and the concentration of sulfate [SO42-] = 0.178 M in GWB according to SP20-4 appendix B.
6 Plot H+ observed in column D aginst H+ free (column F) and get slope of line, 15.428.
7 Correction factor A = log(slope in Figure 2)
8 Input slope and log (slope) in worksheet "sum" to get the average of A from three titrations

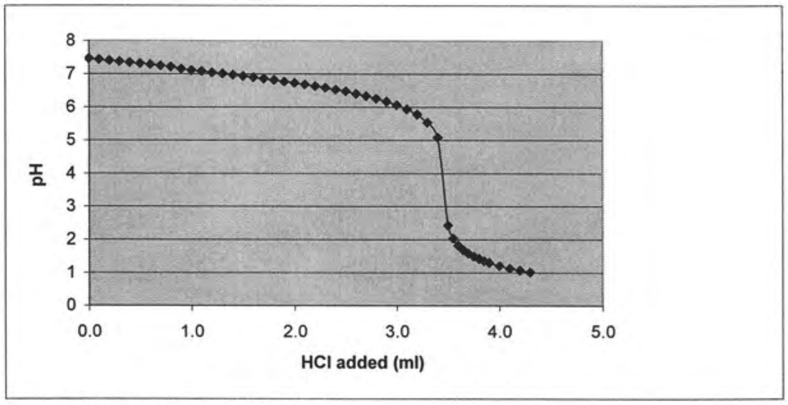


Figure 1. pH versus HCl added

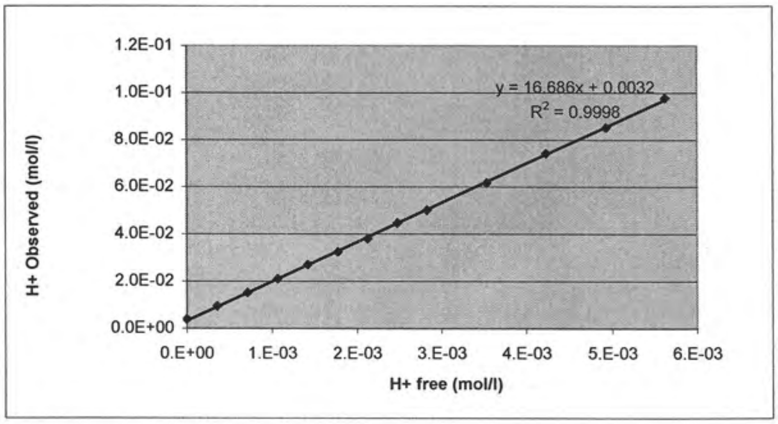


Figure 2. H+ Observed versus H+ Free

slope	log(slope)	R2
16.686	1.222352	0.9998

Brine: GWB
Titrant 1.00M HCl

Temperature:24.85°C Start Time: 10:35am
End Time: 11:48am

Notebook and pg: Wipp-MMMgO-14 p.16

amt added mL	Total Added mL	pH observed	H+ Observed (M)	HCl added (M)	H+ free (M)
0	0	7.47	3.388E-08	0.000E+00	
0.1	0.1	7.43	3.715E-08	1.996E-03	
0.1	0.2	7.4	3.981E-08	3.984E-03	
0.1	0.3	7.37	4.266E-08	5.964E-03	
0.1	0.4	7.33	4.677E-08	7.937E-03	
0.1	0.5	7.3	5.012E-08	9.901E-03	
0.1	0.6	7.27	5.370E-08	1.186E-02	
0.1	0.7	7.23	5.888E-08	1.381E-02	
0.1	0.8	7.2	6.310E-08	1.575E-02	
0.1	0.9	7.17	6.761E-08	1.768E-02	
0.1	1	7.13	7.413E-08	1.961E-02	
0.1	1.1	7.09	8.128E-08	2.153E-02	
0.1	1.2	7.06	8.710E-08	2.344E-02	
0.1	1.3	7.02	9.550E-08	2.534E-02	
0.1	1.4	6.98	1.047E-07	2.724E-02	
0.1	1.5	6.94	1.148E-07	2.913E-02	
0.1	1.6	6.9	1.259E-07	3.101E-02	
0.1	1.7	6.86	1.380E-07	3.288E-02	
0.1	1.8	6.82	1.514E-07	3.475E-02	
0.1	1.9	6.78	1.660E-07	3.661E-02	
0.1	2	6.73	1.862E-07	3.846E-02	
0.1	2.1	6.68	2.089E-07	4.031E-02	
0.1	2.2	6.63	2.344E-07	4.215E-02	
0.1	2.3	6.56	2.754E-07	4.398E-02	
0.1	2.4	6.52	3.020E-07	4.580E-02	
0.1	2.5	6.46	3.467E-07	4.762E-02	
0.1	2.6	6.35	4.467E-07	4.943E-02	
0.1	2.7	6.31	4.898E-07	5.123E-02	
0.1	2.8	6.23	5.888E-07	5.303E-02	
0.1	2.9	6.13	7.413E-07	5.482E-02	
0.05	2.95	6.08	8.318E-07	5.571E-02	
0.05	3	6.02	9.550E-07	5.660E-02	
0.05	3.05	5.92	1.202E-06	5.749E-02	
0.05	3.1	5.86	1.380E-06	5.838E-02	
0.05	3.15	5.8	1.585E-06	5.927E-02	
0.05	3.2	5.69	2.042E-06	6.015E-02	
0.05	3.25	5.56	2.754E-06	6.103E-02	
0.05	3.3	5.39	4.074E-06	6.191E-02	
0.05	3.35	5.12	7.586E-06	6.279E-02	
0.05	3.4	4.5	3.162E-05	0.000E+00	
0.05	3.45	2.44	3.631E-03	9.355E-04	3.570E-04
0.05	3.5	2.02	9.550E-03	1.869E-03	7.133E-04
0.05	3.55	1.8	1.585E-02	2.801E-03	1.069E-03
0.05	3.6	1.66	2.188E-02	3.731E-03	1.424E-03
0.05	3.65	1.55	2.818E-02	4.660E-03	1.778E-03
0.05	3.7	1.46	3.467E-02	5.587E-03	2.132E-03
0.05	3.75	1.39	4.074E-02	6.512E-03	2.485E-03
0.05	3.8	1.32	4.786E-02	7.435E-03	2.837E-03
0.05	3.85	1.27	5.370E-02	8.357E-03	3.189E-03
0.1	3.95	1.18	6.607E-02	1.019E-02	3.890E-03
0.1	4.05	1.1	7.943E-02	1.203E-02	4.589E-03
0.1	4.15	1.03	9.333E-02	1.385E-02	5.286E-03

1+ (1/Ka) x [SO42-] =
2.620E+00

Data location Wipp-MMMgO-14 p.16
Calculation steps:

1 H+ Observed in column D = 10^-pH observed in column C
2 Plot pH observed (column C) against total acid added (column B), Figure 1, and determine the equivalence volume, 3.40 ml
3 H+ added in column E =
(Total added acid in column B - equivalence volume 3.40 ml) x HCl concentration/(Brine volume 50ml + Total volume of added acid in column B)
HCl concentration is given in notebook wipp-FePb-1, p6 and p21.
4 H+ free in column F = H+ added in column E/ value in cell I46 using equation (6) in section 3.3 of the report.
5 Here cell I46 =1+ (1/Ka)x [SO42-] with Ka =10^(-0.9592),
where Ka is given in worksheet "constant", and the concentration of sulfate [SO42-] = 0.178 M in GWB according to SP20-4 appendix B.
6 Plot H+ observed in column D aginst H+ free (column F) and get slope of line, 16.757
7 Correction factor A = log(slope in Figure 2)
8 Input slope and log (slope) in worksheet "sum" to get the average of A from three titrations

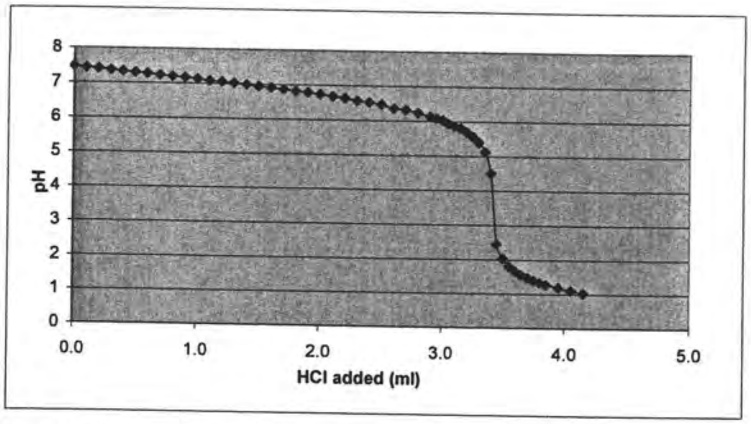


Figure 1. pH versus HCl added

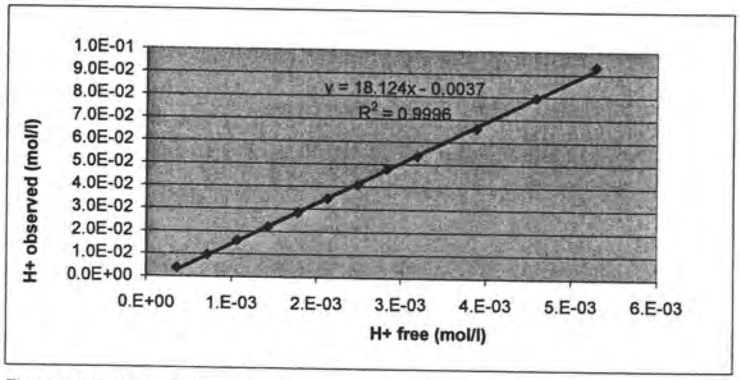


Figure 2. H+ observed versus H+ free

slope	log(slope)	R2
18.124	1.258254	0.9996

Brine: GWB Temperature:24.75°C Start Time: 1:46pm
Titrant 1.00M HCl End Time: 4:04pm
Notebook and pg: Wipp-MMMgO-14 p.17

amt added mL	Total Added mL	pH observed	H+ Observed (M)	HCl added (M)	H+ free (M)		
0	0	7.51	3.090E-08	0.000E+00			
0.1	0.1	7.47	3.388E-08	1.996E-03			
0.1	0.2	7.44	3.631E-08	3.984E-03			
0.1	0.3	7.4	3.981E-08	5.964E-03			
0.1	0.4	7.37	4.266E-08	7.937E-03			
0.1	0.5	7.34	4.571E-08	9.901E-03			
0.1	0.6	7.3	5.012E-08	1.186E-02			
0.1	0.7	7.27	5.370E-08	1.381E-02			
0.1	0.8	7.23	5.888E-08	1.575E-02			
0.1	0.9	7.2	6.310E-08	1.768E-02			
0.1	1	7.16	6.918E-08	1.961E-02			
0.1	1.1	7.13	7.413E-08	2.153E-02			
0.1	1.2	7.09	8.128E-08	2.344E-02			
0.1	1.3	7.05	8.913E-08	2.534E-02			
0.1	1.4	7.01	9.772E-08	2.724E-02			
0.1	1.5	6.97	1.072E-07	2.913E-02			
0.1	1.6	6.93	1.175E-07	3.101E-02			
0.1	1.7	6.89	1.288E-07	3.288E-02			
0.1	1.8	6.84	1.445E-07	3.475E-02			
0.1	1.9	6.8	1.585E-07	3.661E-02			
0.1	2	6.75	1.778E-07	3.846E-02			
0.1	2.1	6.7	1.995E-07	4.031E-02			
0.1	2.2	6.65	2.239E-07	4.215E-02			
0.1	2.3	6.59	2.570E-07	4.398E-02			
0.1	2.4	6.53	2.951E-07	4.580E-02			
0.1	2.5	6.47	3.388E-07	4.762E-02			
0.1	2.6	6.4	3.981E-07	4.943E-02			
0.1	2.7	6.31	4.898E-07	5.123E-02			
0.1	2.8	6.22	6.026E-07	5.303E-02			
0.05	2.85	6.12	7.586E-07	5.393E-02			
0.05	2.9	6.06	8.710E-07	5.482E-02			
0.05	2.95	5.99	1.023E-06	5.571E-02			
0.05	3	5.91	1.230E-06	5.660E-02			
0.05	3.05	5.82	1.514E-06	5.749E-02			
0.05	3.1	5.58	2.630E-06	5.838E-02			
0.05	3.15	5.4	3.981E-06	5.927E-02			
0.05	3.2	5.1	7.943E-06	6.015E-02			
0.05	3.25	4.24	5.754E-05	6.103E-02		1+ (1/Ka) x [SO42-] =	2.620E+00
0.05	3.3	2.38	4.169E-03	0.000E+00	0.000E+00		
0.05	3.35	2.01	9.772E-03	9.372E-04	3.577E-04		
0.05	3.4	1.82	1.514E-02	1.873E-03	7.146E-04		
0.05	3.45	1.68	2.089E-02	2.806E-03	1.071E-03		
0.05	3.5	1.57	2.692E-02	3.738E-03	1.427E-03		
0.05	3.55	1.49	3.236E-02	4.669E-03	1.782E-03		
0.05	3.6	1.41	3.890E-02	5.597E-03	2.136E-03		
0.05	3.65	1.35	4.467E-02	6.524E-03	2.490E-03		
0.05	3.7	1.3	5.012E-02	7.449E-03	2.843E-03		
0.05	3.75	1.25	5.623E-02	8.372E-03	3.195E-03		
0.05	3.8	1.2	6.310E-02	9.294E-03	3.547E-03		
0.05	3.85	1.16	6.918E-02	1.021E-02	3.898E-03		
0.05	3.9	1.13	7.413E-02	1.113E-02	4.248E-03		
0.05	3.95	1.09	8.128E-02	1.205E-02	4.598E-03		
0.05	4	1.06	8.710E-02	1.296E-02	4.947E-03		
0.05	4.05	1.03	9.333E-02	1.388E-02	5.295E-03		

Data location: Wipp-MMMgO-14 p.17
Calculation steps:

1. H+ Observed in column D = 10^-pH observed in column C
2. Plot pH observed (column C) against total acid added (column B), Figure 1, and determine the equivalence volume, 3.30 ml
3. H+ added in column E =
   (Total added acid in column B - equivalence volume 3.30 ml) x HCl concentration/(Brine volume 50ml + Total volume of added acid in column B)
   HCl concentration is given in notebook wipp-FePb-1, p6 and p21.
4. H+ free in column F = H+ added in column E/ value in cell H43 using equation (6) in section 3.3 of the report.
5. Here cell H43 =1+ (1/Ka)x [SO42-] with Ka =10^(-0.9592),
   where Ka is given in worksheet "constant", and the concentration of sulfate [SO42-] = 0.178 M in ERDA-6 according to SP20-4 appendix B.
6. Plot H+ observed in column D aginst H+ free (column F) and get slope of line, 15.622.
7. Correction factor A = log(slope in Figure 2)
8. Input slope and log (slope) in worksheet "sum" to get the average of A from three titrations

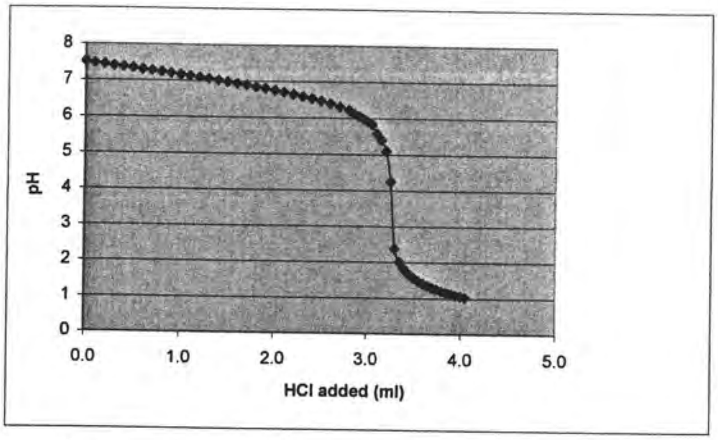


Figure 1. pH versus HCl added

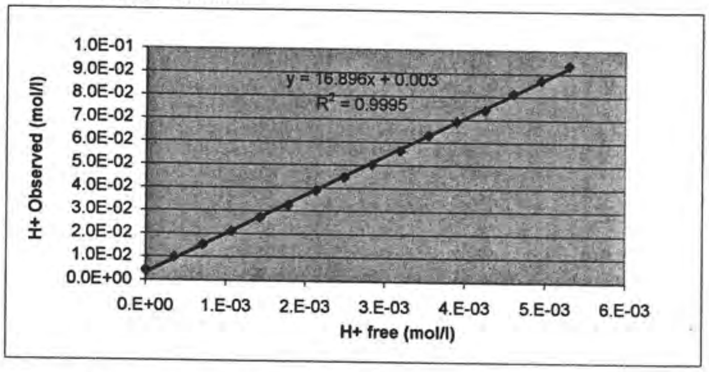


Figure 2. H+ observed versus H+ free

slope	log(slope)	R2
16.896	1.227784	0.9995

Brine: 1MgCl2 + 3. Temperature:24.95'C   Start Time: 2:30pm
Titrant .01M HCl   End Time: 4:45pm
Data location: Wipp-MMMgO-14 p.18

amt added mL	Total Added acid mL	pH observed	H+ observed (M)	H+ added (M)
0	0	6.14	7.24436E-07	0
0.025	0.025	6.04	9.12011E-07	4.9975E-06
0.025	0.05	5.92	1.20226E-06	9.99E-06
0.025	0.075	5.82	1.51356E-06	1.4978E-05
0.025	0.1	5.64	2.29087E-06	1.996E-05
0.025	0.125	5.56	2.75423E-06	2.4938E-05
0.025	0.15	5.46	3.46737E-06	2.991E-05
0.025	0.175	5.37	4.2658E-06	3.4878E-05
0.025	0.2	5.26	5.49541E-06	3.9841E-05
0.025	0.225	5.17	6.76083E-06	4.4798E-05
0.025	0.25	5.02	9.54993E-06	4.9751E-05
0.025	0.275	4.94	1.14815E-05	5.4699E-05
0.025	0.3	4.87	1.34896E-05	5.9642E-05
0.025	0.325	4.77	1.69824E-05	6.458E-05
0.025	0.35	4.64	2.29087E-05	6.9513E-05
0.025	0.375	4.5	3.16228E-05	7.4442E-05
0.025	0.4	4.34	4.57088E-05	7.9365E-05
0.025	0.425	4.15	7.07946E-05	8.4284E-05
0.025	0.45	3.96	0.000109648	8.9197E-05
0.025	0.475	3.8	0.000158489	9.4106E-05
0.025	0.5	3.66	0.000218776	9.901E-05
0.025	0.525	3.5	0.000316228	0.00010391
0.025	0.55	3.45	0.000354813	0.0001088
0.025	0.575	3.38	0.000416869	0.00011369
0.025	0.6	3.31	0.000489779	0.00011858
0.05	0.65	3.2	0.000630957	0.00012833
0.05	0.7	3.11	0.000776247	0.00013807
0.05	0.75	3.03	0.000933254	0.00014778
0.05	0.8	2.97	0.001071519	0.00015748
0.05	0.85	2.91	0.001230269	0.00016716
0.05	0.9	2.86	0.001380384	0.00017682
0.1	1	2.78	0.001659587	0.00019608
0.1	1.1	2.7	0.001995262	0.00021526
0.1	1.2	2.64	0.002290868	0.00023438
0.1	1.3	2.59	0.002570396	0.00025341
0.1	1.4	2.55	0.002818383	0.00027237
0.1	1.5	2.5	0.003162278	0.00029126
0.2	1.7	2.43	0.003715352	0.00032882
0.2	1.9	2.37	0.004265795	0.00036609
0.2	2.1	2.33	0.004677351	0.00040307
0.2	2.3	2.28	0.005248075	0.00043977
0.3	2.6	2.22	0.006025596	0.0004943
0.3	2.9	2.1	0.007943282	0.0005482

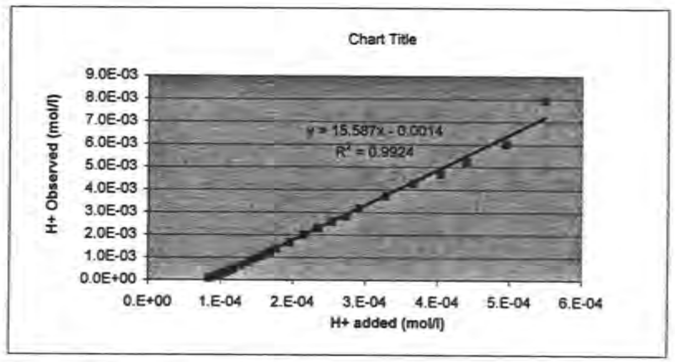


Figure 1. H+ Observed versus H+ added

slope	log(slope)	R2
15.587	1.192763	0.9924

Data location: Wipp-MMMgO-14 p.18
Calculation steps

1 H+ Observed in column D = 10^- pH observed in column C
2 H+ added in column E =
Total added acid in column B x HCl concentration/(Brine volume 50ml + Total added acid in cloumn B)
HCl concentration is given in notebook wipp-mmmgo-14 p18.
3 Plot H+ observed in column D aginst H+ added (column E) and get slope of line 15.587 . Note, not all of the data was used. The cyan bar above indicates where the data set used in the regression begins.
4 Correction factor A = log(slope)
5 Input slope and log (slope) in datasheet "sum" to get the average of A from three titrations

Brine: 1MgCl2 + 3.6M NaCl Temperature:24.90'C Start Time: 9:00am
Titrant .01M HCl End Time: 11:12am
Data location: Wipp-MMMgO-14 p.19

amt. added (mL)	Total added acid (mL)	pH observed	H+ observed (M)	H+ added (M)
0	0	6.12	7.58578E-07	0
0.025	0.025	6	0.000001	4.9975E-06
0.025	0.05	5.89	1.28825E-06	9.99001E-06
0.025	0.075	5.75	1.77828E-06	1.49775E-05
0.025	0.1	5.64	2.29087E-06	1.99601E-05
0.025	0.125	5.52	3.01995E-06	2.49377E-05
0.025	0.15	5.41	3.89045E-06	2.99103E-05
0.025	0.175	5.3	5.01187E-06	3.48779E-05
0.025	0.2	5.19	6.45654E-06	3.98406E-05
0.025	0.225	5.09	8.12831E-06	4.47984E-05
0.025	0.25	4.99	1.02329E-05	4.97512E-05
0.025	0.275	4.89	1.28825E-05	5.46992E-05
0.025	0.3	4.79	1.62181E-05	5.96421E-05
0.025	0.325	4.68	2.0893E-05	6.45802E-05
0.025	0.35	4.57	2.69153E-05	6.95134E-05
0.025	0.375	4.43	3.71535E-05	7.44417E-05
0.025	0.4	4.27	5.37032E-05	7.93651E-05
0.025	0.425	4.1	[redacted]	[redacted]
0.025	0.45	3.93	0.00011749	8.91972E-05
0.025	0.475	3.76	0.00017378	9.4106E-05
0.025	0.5	3.63	0.000234423	9.90099E-05
0.025	0.525	3.52	0.000301995	0.000103909
0.025	0.55	3.42	0.000380189	0.000108803
0.025	0.575	3.35	0.000446684	0.000113693
0.025	0.6	3.27	0.000537032	0.000118577
0.05	0.65	3.16	0.000691831	0.000128332
0.05	0.7	3.06	0.000870964	0.000138067
0.05	0.75	2.99	0.001023293	0.000147783
0.05	0.8	2.93	0.001174898	0.00015748
0.1	0.9	2.81	0.001548817	0.000176817
0.1	1	2.73	0.001862087	0.000196078
0.1	1.1	2.65	0.002238721	0.000215264
0.1	1.2	2.59	0.002570396	0.000234375
0.1	1.3	2.53	0.002951209	0.000253411
0.1	1.4	2.49	0.003235937	0.000272374
0.2	1.6	2.41	0.003890451	0.000310078
0.2	1.8	2.37	0.004265795	0.00034749
0.2	2	2.34	0.004570882	0.000384615
0.2	2.2	2.28	0.005248075	0.000421456
0.2	2.4	2.24	0.005754399	0.000458015
0.2	2.6	2.21	0.00616595	0.000494297
			1	0

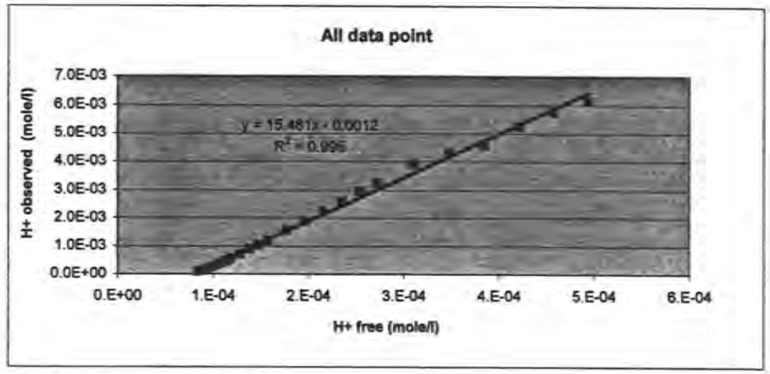


Figure 1. H+ observed versus H+ free

slope	log(slope)	R2
15.481	1.189799	0.995

Data location Wipp-MMMgO-14 p.19
Calculation steps

1 H+ Observed in column D = 10^- pH observed in column C
2 H+ added in column E =
Total added acid in column B x HCl concentration/(Brine volume 50ml + Total added acid in cloumn B)
HCl concentration is given in notebook wipp-mmmgo-14 p18.
3 Plot H+ observed in column D aginst H+ added (column E) and get slope of line 15.481. Note, not all of the data was used. The cyan bar above indicates where the data set used in the regression begins.
4 Correction factor A = log(slope)
5 Input slope and log (slope) in datasheet "sum" to get the average of A from three titrations

Brine: 1MgCl2 + 3.6M NaCl
Titrant .01M HCl

Temperature:24.93'C
Start Time: 12:20pm
End Time: 1:09pm

Notebook and pg.: Wipp-MMMgO-14 p. 20

amt added mL	amt added mL	Total Added acid mL	pH observed	H+ observed (M)	H+ added (M)
0	0	0	6.13	7.4131E-07	0
0.025	0.025	0.025	6.04	9.12011E-07	4.9975E-06
0.025	0.025	0.05	5.92	1.20226E-06	9.99001E-06
0.025	0.025	0.075	5.77	1.69824E-06	1.49775E-05
0.025	0.025	0.1	5.65	2.23872E-06	1.99601E-05
0.025	0.025	0.125	5.56	2.75423E-06	2.49377E-05
0.025	0.025	0.15	5.45	3.54813E-06	2.99103E-05
0.025	0.025	0.175	5.31	4.89779E-06	3.48779E-05
0.025	0.025	0.2	5.21	6.16595E-06	3.98406E-05
0.025	0.025	0.225	5.1	7.94328E-06	4.47984E-05
0.025	0.025	0.25	4.98	1.04713E-05	4.97512E-05
0.025	0.025	0.275	4.89	1.28825E-05	5.46992E-05
0.025	0.025	0.3	4.79	1.62181E-05	5.96421E-05
0.025	0.025	0.325	4.68	2.0893E-05	6.45802E-05
0.025	0.025	0.35	4.53	2.95121E-05	6.95134E-05
0.025	0.025	0.375	4.42	3.80189E-05	7.44417E-05
0.025	0.025	0.4	4.26	5.49541E-05	7.93651E-05
0.025	0.025	0.425	4.11	7.76247E-05	8.42836E-05
0.025	0.025	0.45	3.96	0.000109648	8.91972E-05
0.025	0.025	0.475	3.79	0.000162181	9.4106E-05
0.025	0.025	0.5	3.65	0.000223872	9.90099E-05
0.025	0.025	0.525	3.54	0.000288403	0.000103909
0.025	0.025	0.55	3.44	0.000363078	0.000108803
0.025	0.025	0.575	3.36	0.000436516	0.000113693
0.025	0.025	0.6	3.29	0.000512861	0.000118577
0.025	0.025	0.625	3.23	0.000588844	0.000123457
0.05	0.05	0.675	3.12	0.000758578	0.000133202
0.05	0.05	0.725	3.03	0.000933254	0.000142928
0.05	0.05	0.775	2.96	0.001096478	0.000152634
0.05	0.05	0.825	2.89	0.00128825	0.000162322
0.05	0.05	0.875	2.84	0.00144544	0.00017199
0.1	0.1	0.975	2.74	0.001819701	0.00019127
0.1	0.1	1.075	2.67	0.002137962	0.000210475
0.1	0.1	1.175	2.6	0.002511886	0.000229604
0.1	0.1	1.275	2.56	0.002754229	0.000248659
0.2	0.2	1.475	2.45	0.003548134	0.000286547
0.2	0.2	1.675	2.38	0.004168694	0.000324141
0.2	0.2	1.875	2.32	0.004786301	0.000361446
0.2	0.2	2.075	2.27	0.005370318	0.000398464
0.2	0.2	2.275	2.22	0.006025596	0.000435198

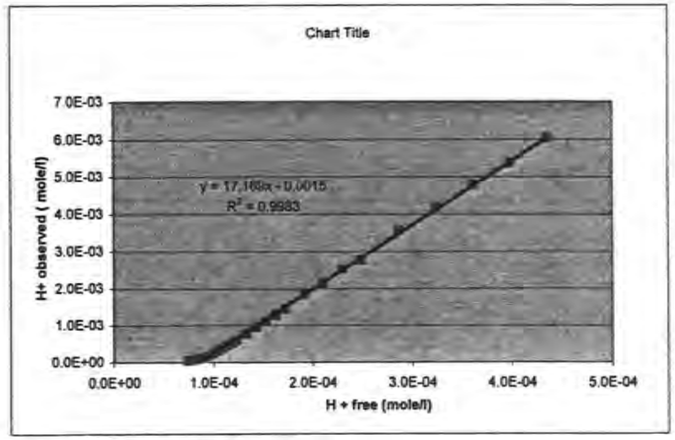


Figure 1. H+ observed versus H+ free

slope	log(slope)	R2
17.169	1.234745	0.9926

Data location: Wipp-MMMgO-14 p. 20

Calculation steps

1. H+ Observed in column D = 10^- pH observed in column C
2. H+ added in column E =
   Total added acid in column B x HCl concentration/(Brine volume 50ml + Total added acid in cloumn B)
   HCl concentration is given in notebook wipp-mmmgo-14 p18.
3. Plot H+ observed in column D aginst H+ added (column E) and get slope of line 17.169. Note, not all of the data was used. The cyan bar above indicates where the data set used in the regression begins.
4. Correction factor A = log(slope)
5. Input slope and log (slope) in datasheet "sum" to get the average of A from three titrations

Brine: EDRA-6 Temperature:25.09'C Start Time: 3:00pm
Titrant 1.00M HCl End Time: 3:57pm
Notebook and pg: Wipp-MMMgO-14 p.12

Amt added mL	Total Added acid mL	pH observed	H+ Observed (M)	H+ added (M)	H+ free (M)	
0	0	7.96	1.096E-08			
0.05	0.05	7.93	1.175E-08			
0.05	0.1	7.9	1.259E-08			
0.05	0.15	7.86	1.380E-08			
0.05	0.2	7.82	1.514E-08			
0.05	0.25	7.79	1.622E-08			
0.05	0.3	7.76	1.738E-08			
0.05	0.35	7.72	1.905E-08			
0.05	0.4	7.67	2.138E-08			
0.05	0.45	7.63	2.344E-08			
0.1	0.55	7.55	2.818E-08			
0.1	0.65	7.45	3.548E-08			
0.1	0.75	7.33	4.677E-08			
0.1	0.85	7.2	6.310E-08			
0.1	0.95	7.04	9.120E-08			
0.05	1	6.93	1.175E-07			
0.05	1.05	6.81	1.549E-07			
0.05	1.1	6.66	2.188E-07			
0.05	1.15	6.44	3.631E-07			
0.05	1.2	6.12	7.586E-07			
0.05	1.25	5.5	3.162E-06			
0.05	1.3	4.08	8.318E-05	0.000E+00		
0.05	1.35	2.52	3.020E-03	9.737E-04	2.904E-04	1+ (1/Ka) x [SO42-] =
0.05	1.4	2.18	6.607E-03	1.946E-03	5.801E-04	3.353512293
0.05	1.45	2	1.000E-02	2.915E-03	8.694E-04	
0.05	1.5	1.87	1.349E-02	3.883E-03	1.158E-03	
0.05	1.55	1.77	1.698E-02	4.850E-03	1.446E-03	
0.05	1.6	1.69	2.042E-02	5.814E-03	1.734E-03	
0.05	1.65	1.62	2.399E-02	6.776E-03	2.021E-03	
0.1	1.75	1.5	3.162E-02	8.696E-03	2.593E-03	
0.1	1.85	1.41	3.890E-02	1.061E-02	3.163E-03	
0.1	1.95	1.34	4.571E-02	1.251E-02	3.731E-03	
0.1	2.05	1.27	5.370E-02	1.441E-02	4.297E-03	
0.1	2.15	1.21	6.166E-02	1.630E-02	4.860E-03	
0.1	2.25	1.16	6.918E-02	1.818E-02	5.422E-03	
0.1	2.35	1.12	7.586E-02	2.006E-02	5.981E-03	
0.1	2.45	1.04	9.120E-02	2.193E-02	6.538E-03	
0.05	2.5	1.02	9.550E-02	2.286E-02	6.816E-03	
0.05	2.55	1	1.000E-01	2.379E-02	7.093E-03	

Data location: Wipp-MMMgO-14 p.12
Calculation steps:

1 H+ Observed in column D = 10^-pH observed in column C
2 Plot pH observed (column C) against total acid added (column B), Figure 1, and determine the equivalence volume, 1.30 ml
3 H+ added in column E =
(Total added acid in column B - equivalence volume 1.30 ml) x HCl concentration/(Brine volume 50ml + Total volume of added acid in column B)
HCl concentration is given in notebook wipp-FePb-1, p6 and p21.
4 H+ free in column F = H+ added in column E/ value in cell G29 using equation (6) in section 3.3 of the report.
5 Here cell G29 =1+ (1/Ka)x [SO42-] with Ka =10^(-1.1490),
where Ka is given in worksheet "constant", and the concentration of sulfate [SO42-] = 0.167 M in ERDA-6 according to SP20-4 appendix B.
6 Plot H+ observed in column D aginst H+ free (column F) and get slope of line, 12.873.
7 Correction factor A = log(slope in Figure 2)
8 Input slope and log (slope) in worksheet "sum" to get the average of A from three titrations

Figure 1 pH vs HCl added

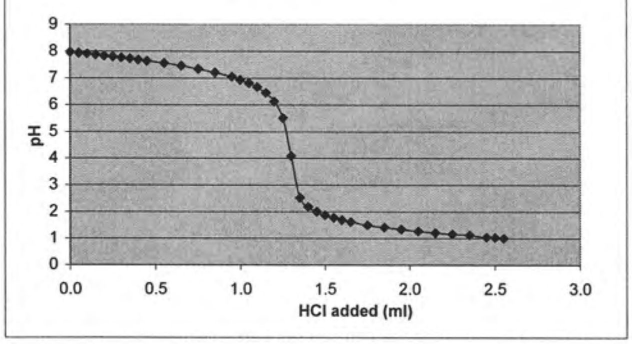
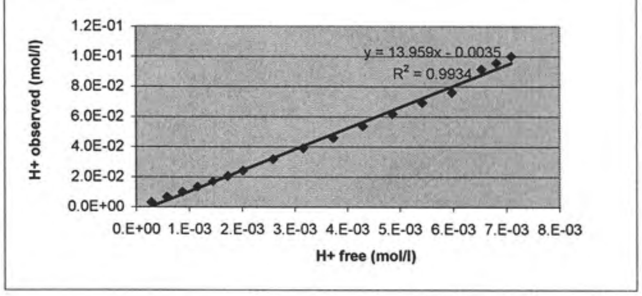


Figure 2 H+ observed vs H+ free



slope	log(slope)	R2
13.959	1.14485431	0.9934

Brine: EDRA-6 Temperature:25.09°C Start Time: 3:00pm
Titrant 1.00M HCl End Time: 3:57pm
Notebook and pg: Wipp-MMMgO-14 p.13

Amt added(ml)	HCl added (ml)	pH Observed	H+ Observed (M)	HCl added (M)	H+ free (M)	
0	0.000	7.90	1.259E-08	0.000E+00		
0.05	0.050	7.86	1.380E-08	9.990E-04		
0.05	0.100	7.86	1.380E-08	1.996E-03		
0.05	0.150	7.83	1.479E-08	2.991E-03		
0.05	0.200	7.79	1.622E-08	3.984E-03		
0.05	0.250	7.76	1.738E-08	4.975E-03		
0.05	0.300	7.72	1.905E-08	5.964E-03		
0.05	0.350	7.68	2.089E-08	6.951E-03		
0.05	0.400	7.64	2.291E-08	7.937E-03		
0.05	0.450	7.60	2.512E-08	8.920E-03		
0.1	0.550	7.51	3.090E-08	1.088E-02		
0.1	0.650	7.41	3.890E-08	1.283E-02		
0.1	0.750	7.29	5.129E-08	1.478E-02		
0.1	0.850	7.15	7.079E-08	1.672E-02		
0.1	0.950	6.98	1.047E-07	1.865E-02		
0.05	1.000	6.87	1.349E-07	1.961E-02		
0.05	1.050	6.74	1.820E-07	2.057E-02		
0.05	1.100	6.56	2.754E-07	2.153E-02		
0.05	1.150	6.30	5.012E-07	2.248E-02		
0.05	1.200	5.82	1.514E-06	2.344E-02		
0.05	1.250	4.98	1.047E-05	0.000E+00		1+ (1/Ka) x [SO42-] =
0.05	1.300	2.77	1.698E-03	9.747E-04	2.906E-04	3.353512293
0.05	1.350	2.28	5.248E-03	1.947E-03	5.807E-04	
0.05	1.400	2.05	8.913E-03	2.918E-03	8.702E-04	
0.05	1.450	1.90	1.259E-02	3.887E-03	1.159E-03	
0.05	1.500	1.78	1.660E-02	4.854E-03	1.448E-03	
0.05	1.550	1.69	2.042E-02	5.820E-03	1.735E-03	
0.05	1.600	1.62	2.399E-02	6.783E-03	2.023E-03	
0.05	1.650	1.55	2.818E-02	7.744E-03	2.309E-03	
0.05	1.700	1.49	3.236E-02	8.704E-03	2.596E-03	
0.05	1.750	1.44	3.631E-02	9.662E-03	2.881E-03	
0.05	1.800	1.39	4.074E-02	1.062E-02	3.166E-03	
0.05	1.850	1.34	4.571E-02	1.157E-02	3.451E-03	
0.05	1.900	1.32	4.786E-02	1.252E-02	3.735E-03	
0.05	1.950	1.28	5.248E-02	1.347E-02	4.018E-03	
0.1	2.050	1.22	6.026E-02	1.537E-02	4.583E-03	
0.1	2.150	1.16	6.918E-02	1.726E-02	5.146E-03	
0.1	2.250	1.11	7.762E-02	1.914E-02	5.707E-03	
0.1	2.350	1.07	8.511E-02	2.101E-02	6.266E-03	
0.1	2.450	1.030	9.333E-02	2.288E-02	6.822E-03	

Data location: Wipp-MMMgO-14 p.13

Calculation steps:

1 H+ Observed in column D = 10^-pH observed in column C
2 Plot pH observed (column C) against total acid added (column B), Figure 1, and determine the equivalence volume, 1.25 ml
3 H+ added in column E =
(Total added acid in column B - equivalence volume 1.25 ml) x HCl concentration/(Brine volume 50ml + Total volume of added acid in column B)
HCl concentration is given in notebook wipp-FePb-1, p6 and p21.
4 H+ free in column F = H+ added in column E/ value in cell G27 using equation (6) in section 3.3 of the report.
5 Here cell G29 =1+ (1/Ka)x [SO42-] with Ka =10^(-1.1490),
where Ka is given in worksheet "constant", and the concentration of sulfate [SO42-] = 0.167 M in ERDA-6 according to SP20-4 appendix B.
6 Plot H+ observed in column D aginst H+ free (column F) and get slope of line, 13.029.
7 Correction factor A = log(slope in Figure 2)
8 Input slope and log (slope) in worksheet "sum" to get the average of A from three titrations

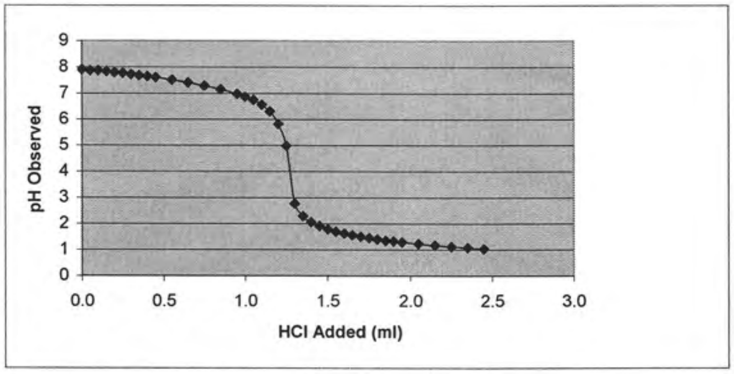


Figure 1. pH observed versus HCl added

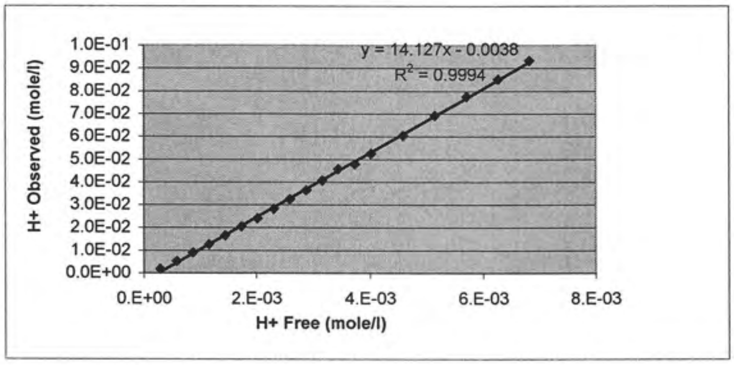


Figure 2. H+ observed versus H+ free

slope	log(slope)	R2
14.127	1.15005	0.9994

Brine: EDRA-6 Temperature:25.09'C Start Time: 3:00pm
Tartan 1.00M HCl End Time: 3:57pm
Notebook and pg: Wipp-MMMgO-14 p.14

amt added (mL)	HCl added (ml)	pH Observed	H+ Observed (M)	HCl added (M)	H+ free (M)
0	0.000	7.93	1.175E-08	0.000E+00	
0.05	0.050	7.90	1.259E-08	9.590E-04	
0.05	0.100	7.83	1.479E-08	1.916E-03	
0.05	0.150	7.79	1.622E-08	2.871E-03	
0.05	0.200	7.72	1.905E-08	3.825E-03	
0.05	0.250	7.67	2.138E-08	4.776E-03	
0.05	0.300	7.63	2.344E-08	5.726E-03	
0.05	0.350	7.59	2.570E-08	6.673E-03	
0.05	0.400	7.54	2.884E-08	7.619E-03	
0.05	0.450	7.50	3.162E-08	8.563E-03	
0.05	0.500	7.45	3.548E-08	9.505E-03	
0.1	0.600	7.34	4.571E-08	1.138E-02	
0.1	0.700	7.21	6.166E-08	1.325E-02	
0.1	0.800	7.03	9.333E-08	1.512E-02	
0.05	0.850	6.96	1.096E-07	1.605E-02	
0.05	0.900	6.85	1.413E-07	1.697E-02	
0.05	0.950	6.72	1.905E-07	1.790E-02	
0.05	1.000	6.53	2.951E-07	1.882E-02	
0.05	1.050	6.25	5.623E-07	1.975E-02	
0.05	1.100	5.73	1.862E-06	2.067E-02	
0.05	1.150	4.77	1.698E-05	2.158E-02	
0.05	1.200	2.64	2.291E-03	0.000E+00	0.000E+00
0.05	1.250	2.22	6.026E-03	9.756E-04	2.909E-04
0.05	1.300	2.00	1.000E-02	1.949E-03	5.813E-04
0.05	1.350	1.86	1.380E-02	2.921E-03	8.711E-04
0.05	1.400	1.75	1.778E-02	3.891E-03	1.160E-03
0.05	1.450	1.66	2.188E-02	4.859E-03	1.449E-03
0.05	1.500	1.59	2.570E-02	5.825E-03	1.737E-03
0.05	1.550	1.52	3.020E-02	6.790E-03	2.025E-03
0.05	1.600	1.45	3.548E-02	7.752E-03	2.312E-03
0.05	1.650	1.42	3.802E-02	8.712E-03	2.598E-03
0.05	1.700	1.37	4.266E-02	9.671E-03	2.884E-03
0.1	1.800	1.29	5.129E-02	1.158E-02	3.454E-03
0.1	1.900	1.22	6.026E-02	1.349E-02	4.022E-03
0.1	2.000	1.17	6.761E-02	1.538E-02	4.588E-03
0.1	2.100	1.11	7.762E-02	1.727E-02	5.151E-03
0.05	2.150	1.09	8.128E-02	1.822E-02	5.432E-03
0.05	2.200	1.07	8.511E-02	1.916E-02	5.713E-03
0.05	2.250	1.05	8.913E-02	2.010E-02	5.992E-03
0.05	2.300	1.03	9.333E-02	2.103E-02	6.272E-03
0.05	2.350	1.01	9.772E-02	2.197E-02	6.551E-03
0.05	2.400	0.99	1.023E-01	2.290E-02	6.829E-03

1+ (1/Ka) x [SO42-] =
3.353512293

Data location Wipp-MMMgO-14 p.14
Calculation steps:

1 H+ Observed in column D = 10^-pH observed in column C
2 Plot pH observed (column C) against total acid added (column B), Figure 1, and determine the equivalence volume, 1.20 ml
3 H+ added in column E =
(Total added acid in column B - equivalence volume 1.20 ml) x HCl concentration/(Brine volume 50ml + Total volume of added acid in column B)
HCl concentration is given in notebook wipp-FePb-1, p6 and p21.
4 H+ free in column F = H+ added in column E/ value in cell G27 using equation (6) in section 3.3 of the report.
5 Here cell G29 =1+ (1/Ka)x [SO42-] with Ka =10^(-1.1490),
where Ka is given in worksheet "constant", and the concentration of sulfate [SO42-] = 0.167 M in ERDA-6 according to SP20-4 appendix B.
6 Plot H+ observed in column D aginst H+ free (column F) and get slope of line, 13.636
7 Correction factor A = log(slope in Figure 2)
8 Input slope and log (slope) in worksheet "sum" to get the average of A from three titrations

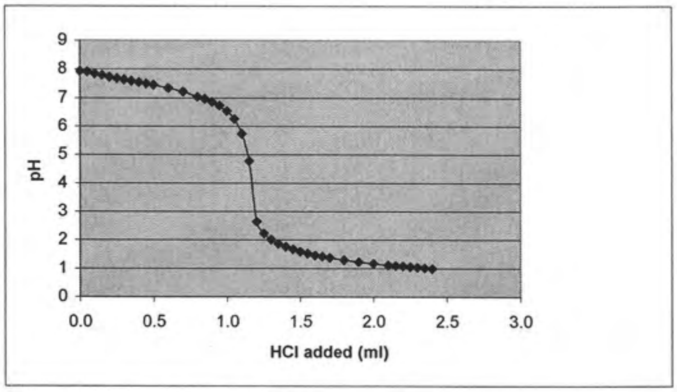


Figure 1. pH versus HCl added

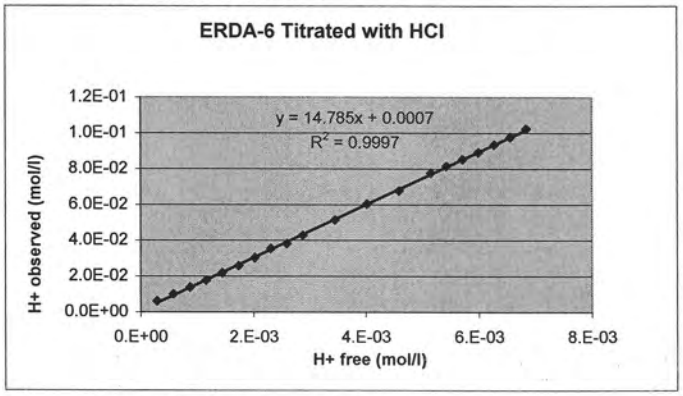
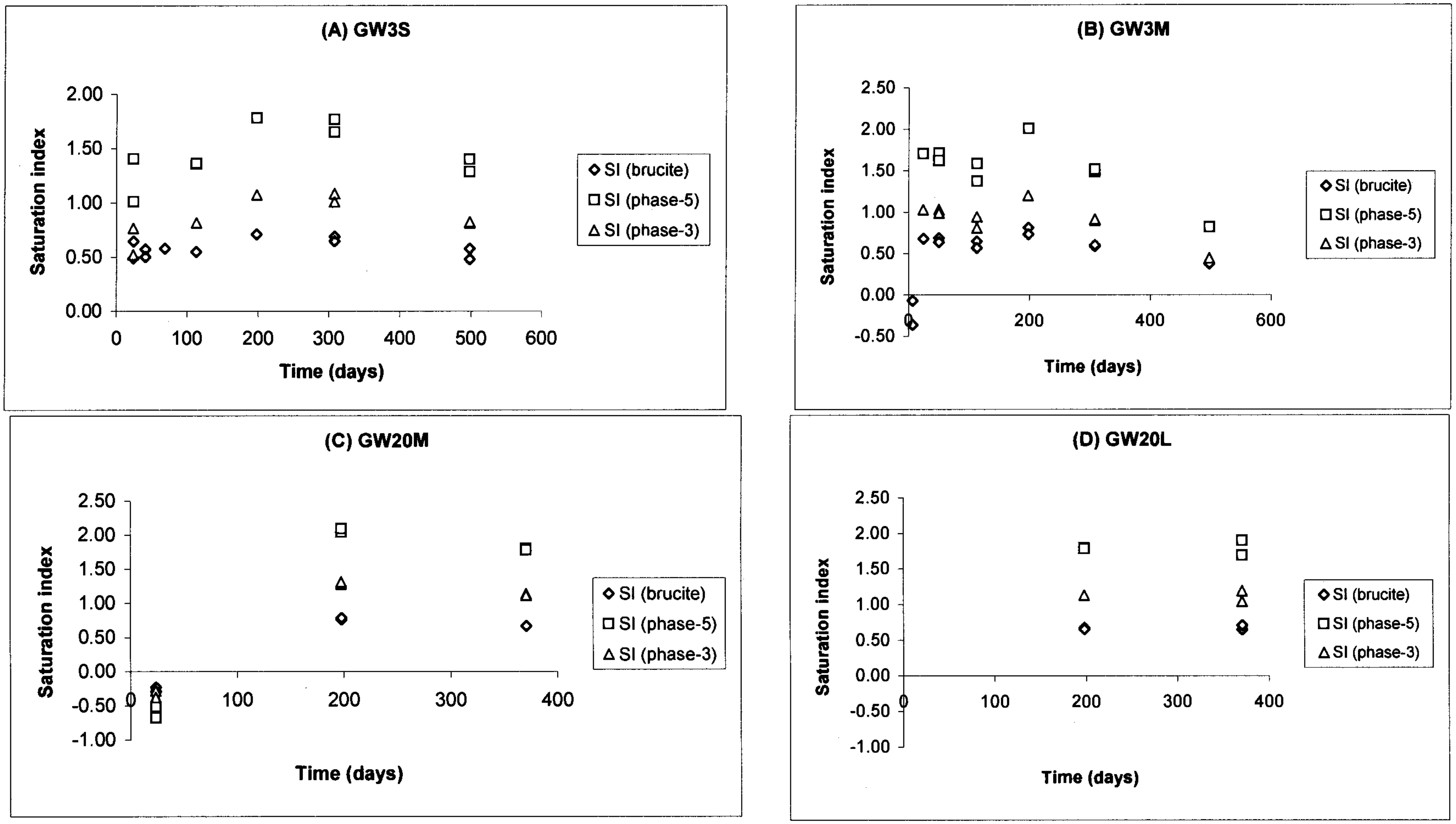
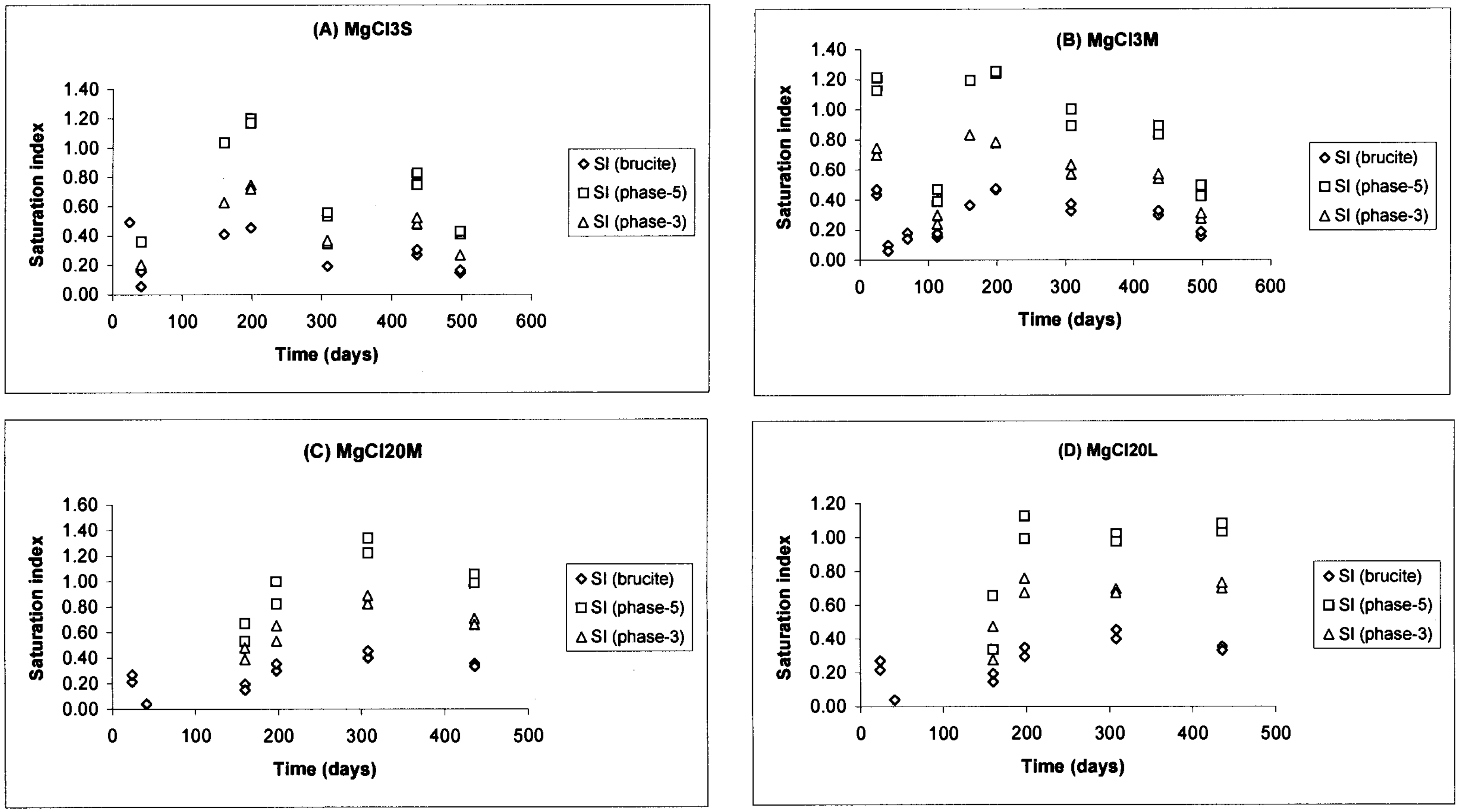


Figure 2. H+ observed versus H+ free

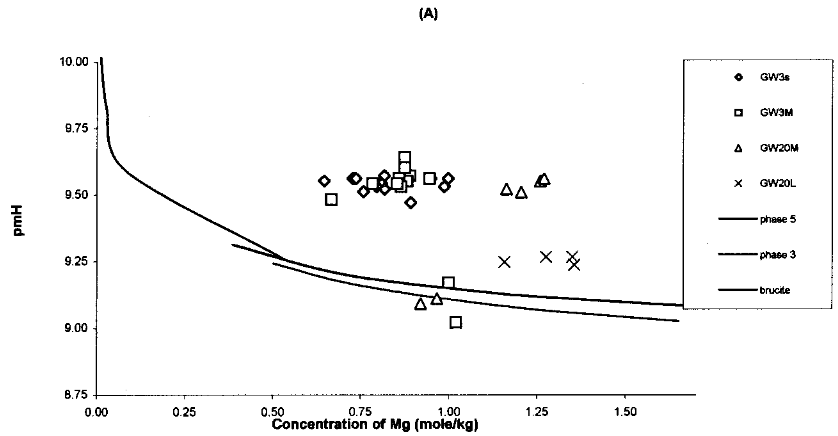
slope	log slope	R2
14.785	1.169821	0.9997



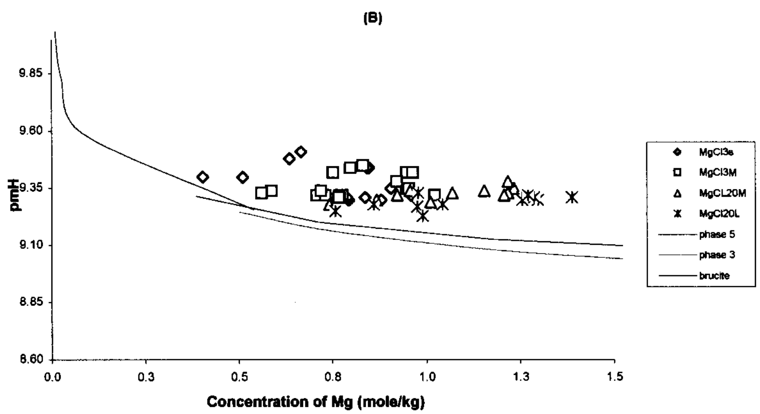
In the above plots, time can be found in columns AM and BG in worksheet "Calculated molality" of this Excel file.
The saturation index can be found in columns BB, BC, BD, BW, BX, and BY in the worksheet "Calculated molality" of this Excel file



In the above plots, time can be found in columns CA and CU in worksheet "Calculated molality" of this Excel file.
The saturation index can be found in columns CP, CQ, CR, DM, DN, and DQ in the worksheet "Calculated molality" of this Excel file

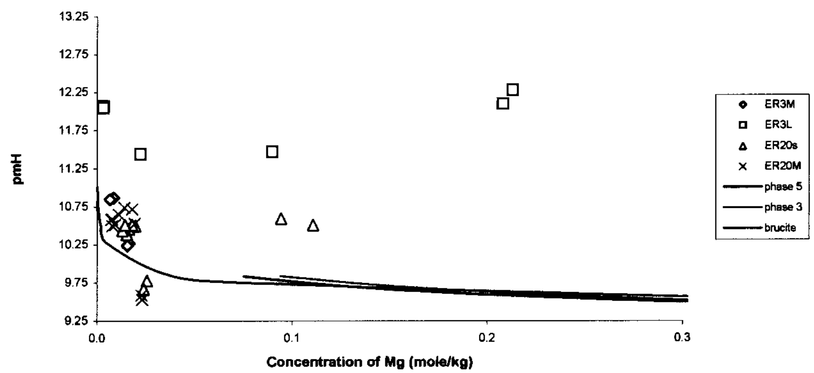


In Fig 30 (A), Mg++ concentration and pmH of GW3S, GW3M, GW20M, GW20L can be found in worksheet "calculated molality" of this Excel file
Mg++ concentration and pmH predicated by EQ6 run for phase-5 equilibrated in GWB brine can be found in Excel file "GWB2(xiong)".
Mg++ concentration and pmH predicated by EQ6 run for phase-3 or brucite equilibrated in GWB brine can be found in Excel file "GWB2(xiong)".
The Excel file "GWB2(xiong)" is part of the memo: Xiong et al, 2009.

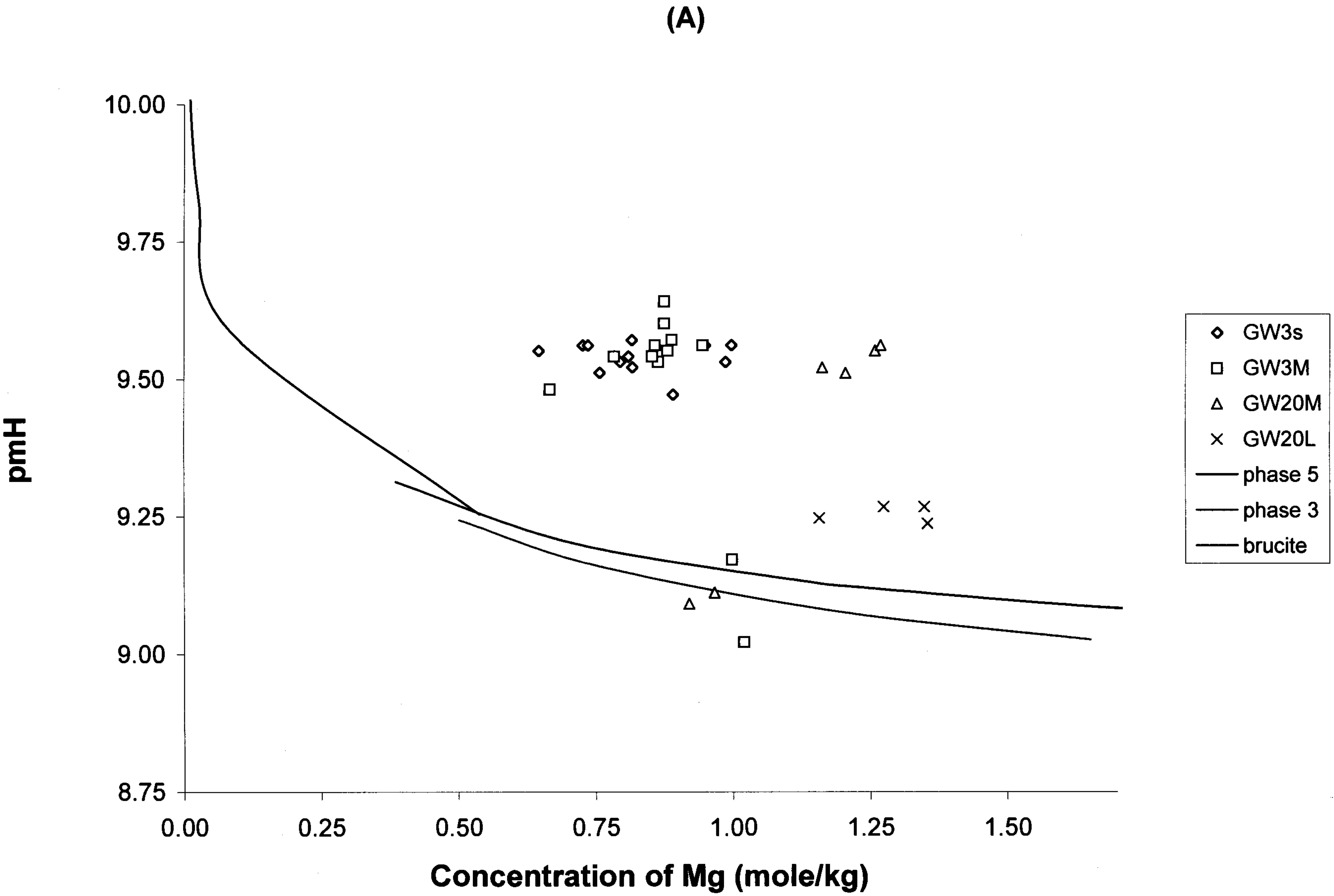


In Fig 30 (B), Mg++ concentration and pmH of MgCl3S, MgCl3M, MgCl20M, MgCl20L can be found in worksheet "calculated molality" of this Excel file
Mg++ concentration and pmH predicated by EQ6 run for phase-5 equilibrated in GWB brine can be found in Excel file "GWB2(xiong)".
Mg++ concentration and pmH predicated by EQ6 run for phase-3 or brucite equilibrated in GWB brine can be found in the Excel file "GWB2(xiong)" respectively.
The Excel file "GWB2(xiong)" is part of the memo: Xiong et al, 2009.

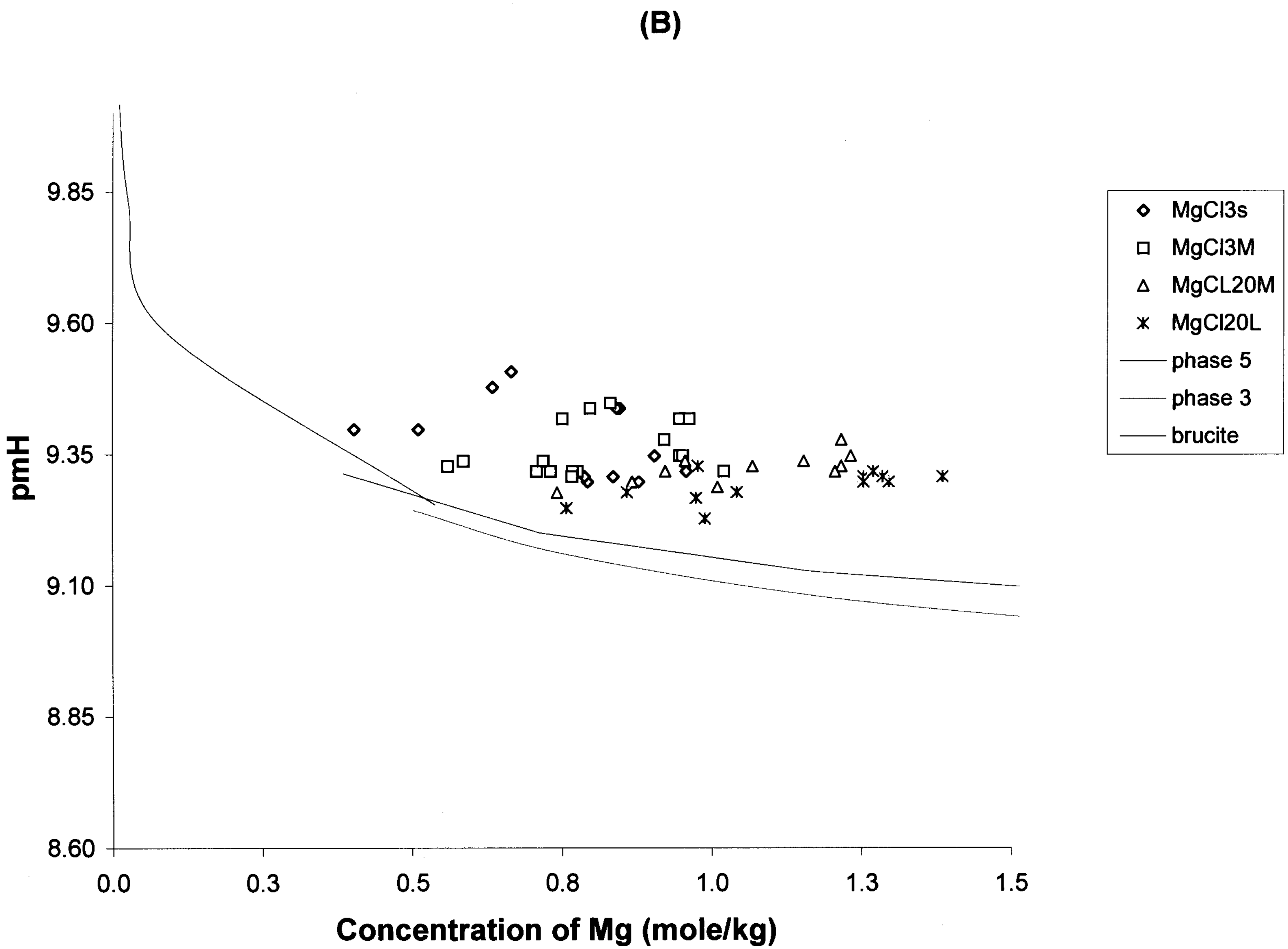
(C)



In Fig 30 (C), Mg++ concentration and pmH of ER3M, ER3L, ER20S, ER20M can be found in worksheet "calculated molality" of this Excel file
Mg++ concentration and pmH predicated by EQ6 run for phase-5 equilibrated in ERDA-6 brine can be found in the Excel file "ERDA-62(xiong)".
Mg++ concentration and pmH predicated by EQ6 run for phase-3 or brucite equilibrated in ERDA-6 brine can be found in the Excel file "ERDA-62(xiong)" respectively.
The Excel file "ERDA-6 2(xiong)" is part of the memo: Xiong et al, 2009.

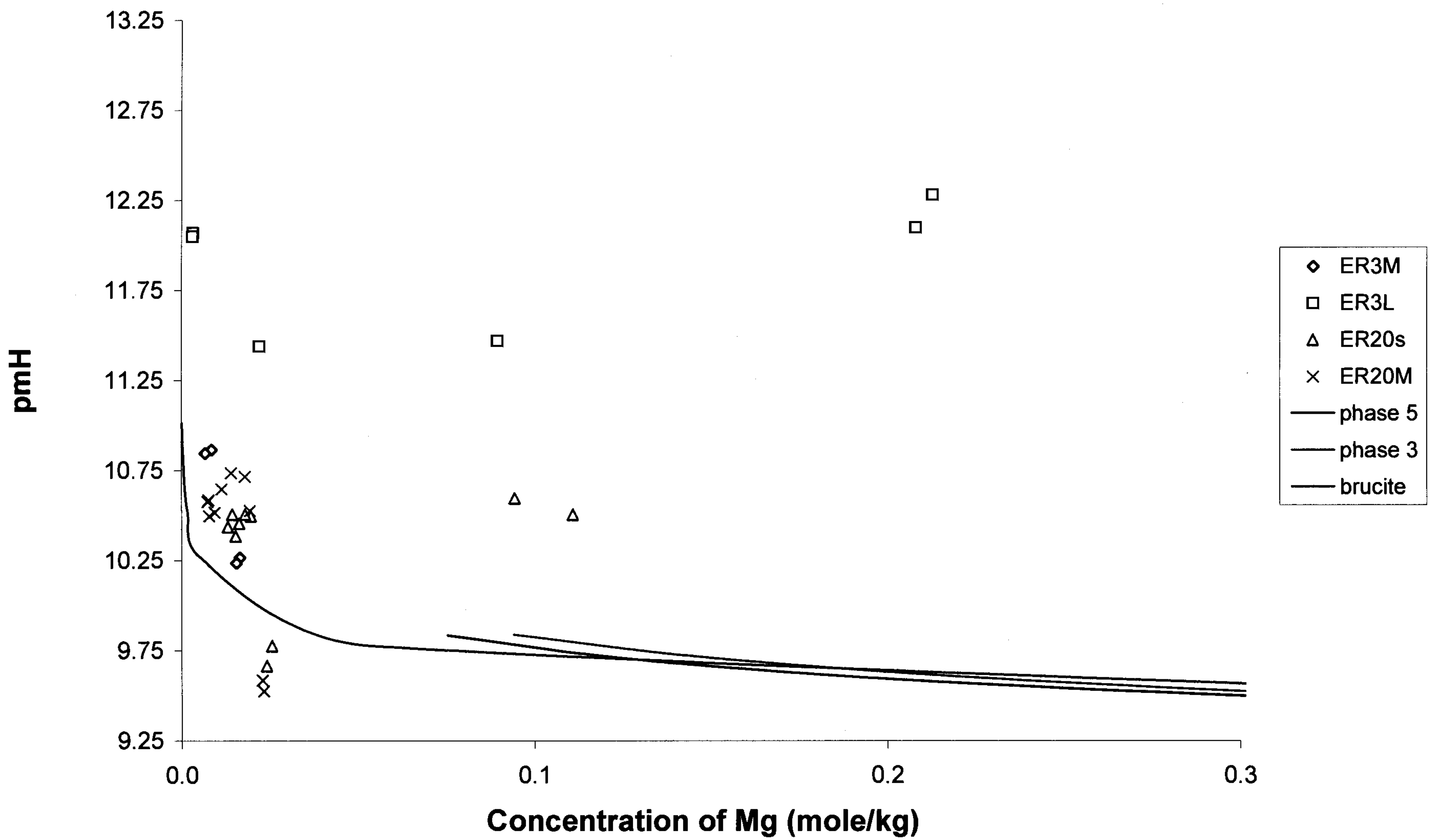


Plots.xls
Datasheet "Fig30(A)"



Plots.xls
Datasheet "Fig 30(B)"

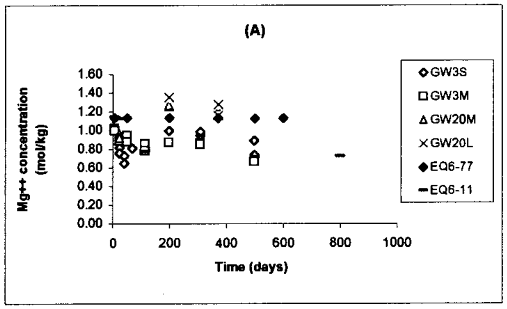
(C)

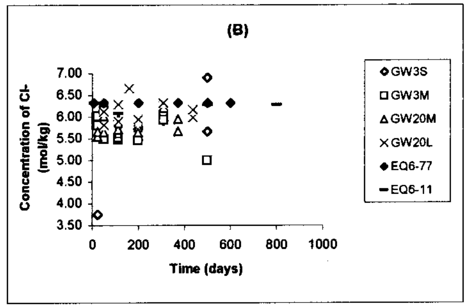


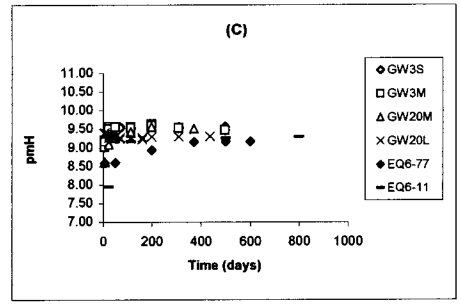
pmH
13.25
12.75
12.25
11.75
11.25
10.75
10.25
9.75
9.25
0.0
0.1
0.2
0.3
Concentration of Mg (mole/kg)
ER3M
ER3L
ER20s
ER20M
phase 5
phase 3
brucite

Arbitrary Time (days)	4/22/2009 User: hdeng EQ3/6, Version 8.0 log Xi - gwb-77.6o	Periclase Moles	Phase-5 Moles	Calcite Moles	Hydromagne 5424 Moles	4/22/2009 User: hdeng EQ3/6, Version 8.0 log Xi - gwb-77.6o	pH - gwb-77.6o	a(w) - gwb-77.6o	Cl- Molality	Mg++ Molality	Ca++ Molality	H+ Molality	Cl- Log Gamma	Mg++ Log Gamma	Ca++ Log Gamma	H+ Log Gamma	pmH
	-99999	1.1629		0.010474	0.00069624	-99999	6.8265	0.720411	6.3203	1.145	0.0051204	1.143E-08	-0.2759	1.1817	0.8863	1.1155	7.94203
	-4.52677	1.1629		0.010456	0.00070971	-4.52677	6.8297	0.720411	6.3203	1.1449	0.0051383	1.135E-08	-0.2759	1.1817	0.8863	1.1155	7.945157
	-3.43998	1.1625		0.010231	0.0006659	-3.43998	6.8671	0.720422	6.3204	1.1445	0.0053635	1.041E-08	-0.2759	1.1817	0.8862	1.1155	7.982549
	-2.37852	1.1587		0.002966	0.003391	-2.37852	7.4625	0.720663	6.3218	1.1362	0.010553	2.649E-09	-0.2759	1.1801	0.8842	1.1144	8.576951
	-2.37717	1.1587		0.0029154	0.0034038	-2.37717	7.4628	0.72067	6.3218	1.1362	0.010555	2.647E-09	-0.2759	1.18	0.8842	1.1144	8.577197
7	-2.30545	1.158			0.0041397	-2.30545	7.4787	0.720845	6.3222	1.1333	0.010698	2.557E-09	-0.2758	1.1787	0.8834	1.1135	8.592218
50	-2.30421	1.1579			0.0041434	-2.30421	7.4867	0.720849	6.3222	1.1333	0.010698	2.511E-09	-0.2758	1.1787	0.8834	1.1135	8.600205
	-2.29738	1.1579			0.0041637	-2.29738	7.5336	0.720853	6.3222	1.1332	0.010699	2.254E-09	-0.2758	1.1786	0.8833	1.1135	8.647046
200	-2.25495	1.1573			0.0042522	-2.25495	7.8262	0.720875	6.3223	1.1328	0.010704	1.149E-09	-0.2758	1.1784	0.8831	1.1134	8.939604
371	-2.2121	1.1568	1.077E-05		0.0042926	-2.2121	8.0505	0.720915	6.3224	1.1323	0.010712	6.86E-10	-0.2758	1.1781	0.8826	1.1131	9.163689
	-2.21163	1.1568	1.362E-05		0.0042926	-2.21163	8.0506	0.720916	6.3224	1.1323	0.010713	6.86E-10	-0.2758	1.178	0.8825	1.1131	9.163689
	-2.21101	1.1567	1.675E-05		0.0042926	-2.21101	8.0506	0.720916	6.3223	1.1323	0.010713	6.86E-10	-0.2758	1.178	0.8825	1.1131	9.163689
	-2.21025	1.1567	2.125E-05		0.0042926	-2.21025	8.0506	0.720917	6.3223	1.1323	0.010713	6.86E-10	-0.2758	1.178	0.8825	1.1131	9.163695
	-2.20928	1.1567	2.682E-05		0.0042926	-2.20928	8.0506	0.720917	6.3223	1.1323	0.010713	6.86E-10	-0.2758	1.178	0.8825	1.1131	9.163689
500	-2.20789	1.1567	3.452E-05		0.0042926	-2.20789	8.0506	0.720917	6.3223	1.1323	0.010714	6.86E-10	-0.2758	1.178	0.8825	1.1131	9.163695
	-2.20452	1.1567	5.399E-05		0.0042926	-2.20452	8.0506	0.720917	6.3223	1.1323	0.010713	6.86E-10	-0.2758	1.178	0.8825	1.1131	9.163695
600	-1.53018	1.1334	0.0093577		0.0042926	-1.53018	8.0523	0.721083	6.3199	1.1289	0.010716	6.847E-10	-0.2758	1.1762	0.8809	1.1122	9.164481
	0.06554	0	0.46276		0.0043001	0.06554	8.1454	0.729691	6.1952	0.95264	0.010898	6.186E-10	-0.2749	1.0819	0.7978	1.0632	9.208611
700																	

	4/22/2009 User: hdeng EQ3/6, Version 8.0 log Xi - gwb-11.6o	Periclase Moles	Brucite Moles	Phase-5 Moles	4/22/2009 User: hdeng EQ3/6, Version 8.0 log Xi - gwb-11.6o	pH - gwb-11.6o	a(w) - gwb-11.6o	Cl- Molality	Mg++ Molality	Ca++ Molality	H+ Molality	Cl- Log Gamma	Mg++ Log Gamma	Ca++ Log Gamma	H+ Log Gamma	pmH
7	-99999	7.8779			-99999	6.8265	0.720411	6.3203	1.145	0.0051204	1.143E-08	-0.2759	1.1617	0.8863	1.1155	7.9420298
24	-1.30103	7.8279		0.017559	-1.30103	8.0538	0.72123	6.3176	1.1258	0.010719	6.836E-10	-0.2758	1.1746	0.8795	1.1114	9.1651852
113	0.36003	5.5869	0.098486	0.87471	0.36003	8.2455	0.737546	6.0812	0.77601	0.011021	5.463E-10	-0.2741	0.9926	0.7187	1.0171	9.2625926
500	0.69358	2.9395	2.2713	1.0645	0.69358	8.2412	0.727753	6.2765	0.71933	0.009735	5.075E-10	-0.2747	1.0458	0.7642	1.0534	9.2945725
	0.76132	2.106	3.052	1.0856	0.76132	8.2408	0.727463	6.2784	0.72098	0.0095916	5.07E-10	-0.2748	1.0459	0.7636	1.0543	9.2950177
800	0.89641	0	5.0251	1.1388	0.89641	8.2396	0.726744	6.2835	0.72556	0.0092306	5.054E-10	-0.2749	1.0463	0.7619	1.0568	9.2963991







Explanation: Except for the data in column A which are arbitrary time, all data from row 3 to row 14 are extracted from EQ6 output file " gwb-77.6o"
Cl- log gamma, H+ log gamma, Mg++ log gamma and aw (water activity) in row 12 are used in worsheet "calculated molality" of this Excel file
As MgO is titrated into the brine, the Cl- log gamma, H+ log gamma, Mg++ log gamma and aw change slightly.
In our calculation, we chose the values for the activity coefficients from the EQ6 outpuf file when phase-5 first appears, row 12.

Except for the data in column A which are arbitrary time, all data from row 17 to row 32 are extracted from EQ6 output file " gwb-11.6o"
Cl- log gamma, H+ log gamma, Mg++ log gamma and aw (water activity) in row 26 are used in worksheet "calculated molality" of this Excel file
In our calculation, we chose the values for the activity coefficients from the EQ6 output file when brucite first appears, row 26.

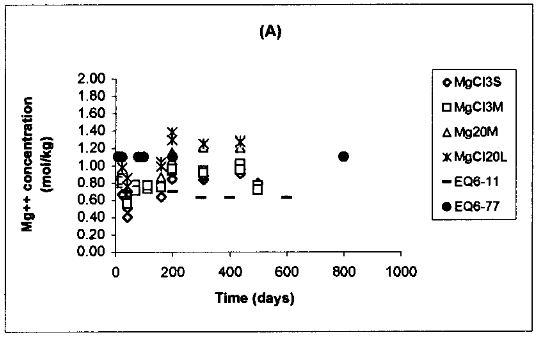
In Fig A, Mg++ concentration of GW3S, GW3M, GW20M, GW20L can be found in worksheet "calculated molality" of this Excell file
Mg++ concentration predicated by EQ6 run for MgO titrated into 77ml and 11 ml of GWB brine can be found in columns K and J above, from EQ6 output files gwb-77.60 and gwb-11.6o respectively

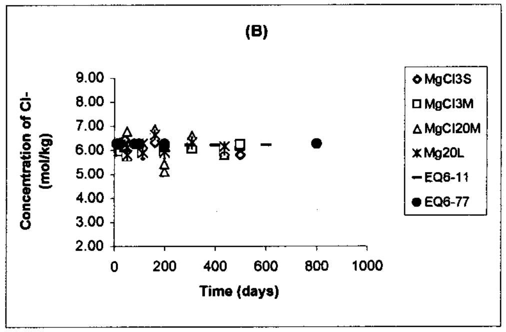
In Fig B, Cl- concentration of GW3S, GW3M, GW20M, GW20L can be found in worksheet "calculated molality" of this Excel file
Cl- concentration predicated by EQ6 run for MgO titrated into 77ml and 11 ml of GWB brine can be found in columns J and I above, from EQ6 output files gwb-77.60 and gwb-11.6o respectively.

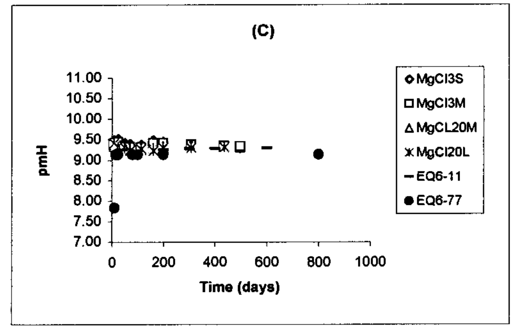
In Fig C, pmH of GW3S, GW3M, GW20M, GW20L can be found in worksheet "calculated molality" of this Excel file
pmH predicated by EQ6 run for MgO titrated into 77ml and 11 ml of GWB brine can be found in columns R and Q above, from EQ6 output files gwb-77.60 and gwb-11.6o respectively

Arbitrary Time (days)	3/18/2009 User: hdeng EQ3/6, Version 8.0 log Xi - sgwbb-77.6o	Periclase Moles	Phase-5 Moles	3/18/2009 User: hdeng EQ3/6, Version 8.0 log Xi - sgwbb-77.6o	pH - sgwbb-77.6o	a(w) - sgwbb-77.6o	Cl- Molality	Mg++ Molality	H+ Molality	Cl- Log Gamma	Mg++ Log Gamma	H+ Log Gamma	pmH
	-99999	1.1555		-99999	6.5845	0.731964	6.2683	1.1054	2.0953E-08	-0.2733	1.1814	1.0942	7.67875379
10	-2.69484	1.1535		-2.69484	6.7385	0.732064	6.2685	1.1042	1.4703E-08	-0.2733	1.1812	1.0941	7.83259404
15	-2.22369	1.1495		-2.22369	8.0444	0.732274	6.2691	1.1015	7.2791E-10	-0.2733	1.1803	1.0935	9.13792231
24	-2.22366	1.1495	1.16E-07	-2.22366	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.13792828
80	-2.22365	1.1495	1.6713E-07	-2.22365	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.13792828
100	-2.22364	1.1495	2.3442E-07	-2.22364	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.13792828
200	-2.22362	1.1495	3.319E-07	-2.22362	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.13792828
	-2.22359	1.1495	5.3087E-07	-2.22359	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.13792828
	-2.22347	1.1495	1.1588E-06	-2.22347	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.13792828
	-2.22315	1.1495	2.927E-06	-2.22315	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.13792828
800	-2.18146	1.1489	0.00024405	-2.18146	8.0444	0.732279	6.2691	1.1014	7.2786E-10	-0.2733	1.1802	1.0935	9.13795215
	0.06277	0	0.45987	0.06277	8.1388	0.741559	6.1398	0.92129	6.577E-10	-0.2721	1.0867	1.0432	9.18197216

	3/18/2009 User: hdeng EQ3/6, Version 8.0 log Xi - sgwbb-11.6o	Periclase Moles	Brucite Moles	Phase-5 Moles	3/18/2009 User: hdeng EQ3/6, Version 8.0 log Xi - sgwbb-11.6o	pH - sgwbb-11.6o	a(w) - sgwbb-11.6o	Cl- Molality	Mg++ Molality	H+ Molality	Cl- Log Gamma	Mg++ Log Gamma	H+ Log Gamma	pmH
	-99999	7.8279			-99999	6.5845	0.731964	6.2683	1.1054	2.0953E-08	-0.2733	1.1814	1.0942	7.678754
	-2.69484	7.8259			-2.69484	6.7385	0.732064	6.2685	1.1042	1.4703E-08	-0.2733	1.1812	1.0941	7.832594
	-2.22369	7.8219			-2.22369	8.0444	0.732274	6.2691	1.1015	7.2791E-10	-0.2733	1.1803	1.0935	9.137922
24	-2.22366	7.8219		1.16E-07	-2.22366	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.137928
	-2.22365	7.8219		1.6713E-07	-2.22365	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.137928
	-2.22364	7.8219		2.3442E-07	-2.22364	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.137928
	-2.22362	7.8219		3.319E-07	-2.22362	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.137928
	-2.22359	7.8219		5.3087E-07	-2.22359	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.137928
	-2.22347	7.8219		1.1588E-06	-2.22347	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.137928
	-2.22315	7.8219		2.927E-06	-2.22315	8.0444	0.732274	6.2691	1.1015	7.279E-10	-0.2733	1.1803	1.0935	9.137928
	-2.18146	7.8213		0.00024405	-2.18146	8.0444	0.732279	6.2691	1.1014	7.2786E-10	-0.2733	1.1802	1.0935	9.137952
41	0.38501	5.4012	0.014827	0.96249	0.38501	8.2682	0.752603	5.9823	0.6995	5.6143E-10	-0.2706	0.9747	0.9825	9.250704
200	0.38511	5.4007	0.015256	0.96253	0.38511	8.2682	0.752601	5.9824	0.69949	5.6142E-10	-0.2706	0.9748	0.9825	9.250712
300	0.7265	2.5007	2.3879	1.1735	0.7265	8.265	0.741668	6.2149	0.62834	5.1466E-10	-0.2713	1.0404	1.0235	9.28848
400	0.72668	2.4985	2.39	1.1735	0.72668	8.265	0.741668	6.2149	0.62834	5.1466E-10	-0.2713	1.0404	1.0235	9.28848
600	0.89365	0	4.7305	1.2367	0.89365	8.2651	0.74167	6.2163	0.62779	5.1453E-10	-0.2713	1.0405	1.0235	9.288589







Explanation: Except for the data in column A which are arbitrary time, all data from row 3 to row 21 are extracted from EQ6 output file "sgwb-77.6o"
Cl- log gamma, H+ log gamma, Mg++ log gamma and aw (water activity) in row 6 are used in data sheet "calculated molality" of this Excel file
As MgO is titrated into the brine, the Cl- log gamma, H+ log gamma, Mg++ log gamma and aw (water activity) change slightly.
In our calculation, we chose the values for the activity coefficients when phase-5 first appears, row 6

Except for the data in column A which are arbitrary time, all data from row 17 to row 32 are extracted from EQ6 output file "sgwb-11.6o"
Cl- log gamma, H+ log gamma, Mg++ log gamma and aw in row 28 are used in data sheet "calculated molality" of this Excel file
In our calculation, we chose the values for the activity coefficients from the EQ6 output file when brucite first appears, i.e. row 28

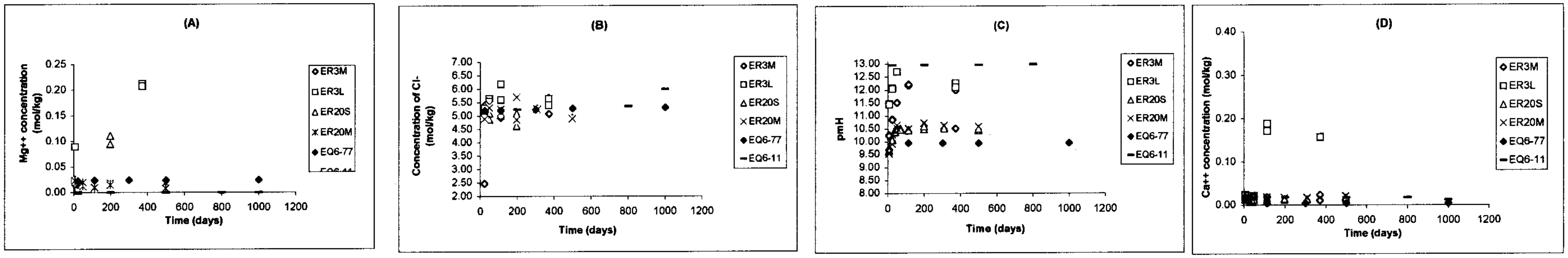
In Fig A, the Mg++ concentration of MgCl3S, MgCl3M, MgCl20M, MgCl20L can be found in worksheet "calculated molality" of this Excel file
Mg++ concentration predicated by EQ6 run for MgO titrated into 77ml and 11 ml of simplified GWB brine can be found in column I above, from EQ6 output files sgwb-77.6o and sgwb-11.6o respectively.

In Fig B, Cl- concentration of MgCl3S, MgCl3M, MgCl20M, MgCl20L can be found in data sheet "calculated molality" of this Excel file
Cl concentration predicated by EQ6 run for MgO titrated into 77ml and 11 ml of simplified GWB brine can be found in columns H and I above, from from EQ6 output files sgwb-77.6o and sgwb-11.6o respectively.

In Fig C, pmH of MgCl3S, MgCl3M, MgCl20M, MgCl20L can be found in data sheet "calculated molality" of this Excel file
pmH predicated by EQ6 run for MgO titrated into 77ml and 11 ml of simplified GWB brine can be found in columns N and O above, from from EQ6 output files sgwb-77.6o and sgwb-11.6o respectively.

	4/29/2009 User: hdeng EQ3/6, Version 8.0			PM 4/29/2009 User: hdeng											
Arbitrary Time (days)	log Xi - erdca-12.6o	Brucite Moles	Periclase Moles	log Xi - erdca-12.6o	pH - erdca-12.6o	a(w) - erdca-12.6o	Cl- Molality	Ca++ Molality	Mg++ Molality	H+ Molality	Cl- Log Gamma	Ca++ Log Gamma	Mg++ Log Gamma	H+ Log Gamma	pmH
24	-99999	0.0213	7.8437	-99999	12.2096	0.788766	5.2037	0.018241	2.2171E-08	1.0915E-13	-0.2664	0.3294	0.5502	0.7524	12.96198
200	-0.39794	0.4213	7.4437	-0.39794	12.2076	0.78694	5.2416	0.017991	2.18E-08	1.0757E-13	-0.2666	0.3413	0.5634	0.7607	12.96831
500	-0.09691	0.8213	7.0437	-0.09691	12.2057	0.785084	5.28	0.01774	2.1428E-08	1.06E-13	-0.2668	0.3533	0.5768	0.769	12.97469
	0.07918	1.2213	6.6437	0.07918	12.2037	0.783197	5.3189	0.017488	2.1056E-08	1.0442E-13	-0.267	0.3656	0.5905	0.7775	12.98122
800	0.20412	1.6213	6.2437	0.20412	12.2017	0.781277	5.3584	0.017236	2.0684E-08	1.0283E-13	-0.2672	0.3781	0.6044	0.7862	12.98788
	0.30103	2.0213	5.8437	0.30103	12.1997	0.779324	5.3986	0.016982	2.0311E-08	1.0125E-13	-0.2674	0.3908	0.6185	0.795	12.9946
	0.38021	2.4213	5.4437	0.38021	12.1979	0.777635	5.4332	0.016763	1.9993E-08	9.989E-14	-0.2676	0.4017	0.6307	0.8026	13.00048
	0.44716	2.8213	5.0437	0.44716	12.1968	0.775624	5.4744	0.016434	1.9533E-08	9.808E-14	-0.2678	0.4148	0.6452	0.8116	13.00842
	0.50515	3.2213	4.6437	0.50515	12.1958	0.773577	5.5183	0.016105	1.9076E-08	9.6271E-14	-0.268	0.428	0.66	0.8207	13.0165
	0.5563	3.6213	4.2437	0.5563	12.1947	0.771495	5.5588	0.015775	1.862E-08	9.4463E-14	-0.2682	0.4415	0.675	0.8301	13.02474
	0.60206	4.0213	3.8437	0.60206	12.1936	0.769375	5.6019	0.015446	1.8167E-08	9.2656E-14	-0.2684	0.4553	0.6903	0.8396	13.03313
	0.64345	4.4213	3.4437	0.64345	12.1925	0.767216	5.6457	0.015118	1.7716E-08	9.0851E-14	-0.2686	0.4692	0.7058	0.8492	13.04167
	0.68124	4.8213	3.0437	0.68124	12.1914	0.765019	5.6903	0.01479	1.7267E-08	8.9048E-14	-0.2688	0.4834	0.7217	0.859	13.05038
	0.716	5.2213	2.6437	0.716	12.1903	0.762782	5.7355	0.014462	1.6821E-08	8.7247E-14	-0.269	0.4979	0.7378	0.869	13.05925
	0.74819	5.6213	2.2437	0.74819	12.1892	0.760504	5.7814	0.014135	1.6378E-08	8.5449E-14	-0.2693	0.5126	0.7542	0.8791	13.06829
	0.77815	6.0213	1.8437	0.77815	12.1881	0.758183	5.8281	0.013809	1.5938E-08	8.3654E-14	-0.2695	0.5276	0.7709	0.8894	13.07751
	0.80618	6.4213	1.4437	0.80618	12.187	0.75582	5.6756	0.013484	1.55E-08	8.1864E-14	-0.2697	0.5429	0.7879	0.8999	13.08691
	0.83251	6.8213	1.0437	0.83251	12.1859	0.753412	5.9238	0.013159	1.5067E-08	8.0077E-14	-0.2699	0.5584	0.8052	0.9106	13.09649
	0.85733	7.2213	0.6437	0.85733	12.1848	0.750958	5.9729	0.012836	1.4636E-08	7.8296E-14	-0.2701	0.5743	0.8228	0.9215	13.10626
	0.86852	7.4092	0.45581	0.86852	12.1844	0.749911	5.9937	0.012697	1.4452E-08	7.7534E-14	-0.2702	0.581	0.8303	0.9261	13.11051
	0.88081	7.6213	0.2437	0.88081	12.1853	0.749894	5.9933	0.012654	1.4397E-08	7.7381E-14	-0.2703	0.5807	0.8302	0.9261	13.11137
1000	0.69452	7.865	0	0.89452	12.1863	0.749875	5.9928	0.012605	1.4335E-08	7.7205E-14	-0.2703	0.5805	0.8301	0.9261	13.11235

	4/22/2009 User: hdeng EQ3/6, Version 8.0			PM 4/22/2009 User: hdeng											
Arbitrary Time (days)	log Xi - erdca-78.6o	Periclase Moles	Brucite Moles	log Xi - erdca-78.6o	pH - erdca-78.6o	a(w) - erdca-78.6o	Cl- Molality	Ca++ Molality	Mg++ Molality	H+ Molality	Cl- Log Gamma	Ca++ Log Gamma	Mg++ Log Gamma	H+ Log Gamma	pmH
24	-99999	1.1579		-99999	6.755	0.788843	5.1987	0.007694	0.021279	3.077E-08	-0.2666	0.3472	0.5634	0.7569	7.511873
113	-2.64152	1.1556	1.196E-07	-2.64152	9.1921	0.788996	5.1986	0.003585	0.023317	1.1253E-10	-0.2666	0.3447	0.5629	0.7566	9.948732
300	-0.39794	0.7579	0.39772	-0.39794	9.185	0.787157	5.2361	0.003609	0.023484	1.1224E-10	-0.2668	0.3565	0.5762	0.7649	9.949852
500	-0.09691	0.3579	0.79771	-0.09691	9.1776	0.785277	5.2744	0.003633	0.023653	1.1194E-10	-0.267	0.3686	0.5898	0.7734	9.951015
1000	0.06367	0	1.1556	0.06367	9.171	0.783567	5.3091	0.003655	0.023808	1.1166E-10	-0.2672	0.3796	0.6021	0.7811	9.952102



Explanation: Except for the data in column A which are arbitrary time, all data from row 3 to row 21 are extracted from the EQ6 output file "erdca-12.6o"
Cl- log gamma, H+ log gamma, Mg++ log gamma and aw (water activity) in row 3 are used in worksheet "calculated molality" of this Excal file
As MgO is titrated into the brine, the Cl- log gamma, H+ log gamma, Mg++ log gamma and aw change slightly.
In our calculation, we chose the values for the activity coefficients from the EQ6 output file when brucite first appears, row 3

Except for the data in column A which are arbitrary time, all data from row 17 to row 32 are extracted from EQ6 output file "erdca-78.6o"
Cl- log gamma, H+ log gamma, Mg++ log gamma and aw (water activity) in row 27 are used in worksheet "calculated molality" of this Excel file
In our calculation, we chose the values for the activity coefficients from the EQ6 output file when brucite first appears, row 27

In Fig A, the Mg++ concentration of ER3M, ER3L, ER20S, ER20M can be found in worksheet "calculated molality" of this Excel file
Mg++ concentration predicated by EQ6 run for MgO titrated into 77ml and 11 ml of ERDA-6 brine can be found in column J above, from files erdca-12.6o and erdca-78.6o respectively

In Fig B, Cl- concentration of ER3M, ER3L, ER20S, ER20M can be found in data sheet "calculated molality" of this Excel file
Cl concentration prediceted by EQ6 run for MgO titrated into 77ml and 11 ml of ERDA-6 brine can be found in column H above, from files erdca-12.6o and erdca-78.6o respectively

In Fig C, pmH of ER3M, ER3L, ER20S, ER20M can be found in data sheet "calculated molality" of this Excel file
pmH predicated by EQ6 run for MgO titrated into 77ml and 11 ml of ERDA-6 brine can be found in column P, from files erdca-12.6o and erdca-78.6o respectively

In Fig D, Ca++ concentration of ER3M, ER3L, ER20S, ER20M can be found in data sheet "calculated molality" of this Excel file
Ca concentration predicated by EQ6 run for MgO titrated into 77ml and 11 ml of ERDA-6 brine can be found in column I, from files erdca-12.6o and erdca-78.6o respectively

77ml	of 1M MgCl2 + 3.6M NaCl	MW			
		Mg (g/mol)	24.305		
3.1 g	of MgO	Na (g/mol)	22.989768		
MW MgCl2 (g/mole)	95.2104	Cl (g/mol)	35.4527		
MW NaCl (g/mole)	58.44247	O (g/mol)	15.9994		
MW MgO (g/mole)	38.98917				
Density (simplified GWB) (g/ml)	1.1992 (WIPP-MgO-CBD-26, p82)				
salt/L of brine (g/L)	Water in 77ml of brine (g)	MgO mole/kg of water		molality to molarity	
305.6033	68.8069	1.1555		1.119073048	

Input: Reaction condition: 3.1g of MgO hydrated in 77ml of simplified GWB (i.e. 1M MgCl2 +3.6 M NaCl)
Simplified GWB density = 1.1992 g/ml recorded in WIPP-MgO-CBD-26, p82

Calculation
Molecular weight of MgCl2 in cell B4 = Molecular weight of Mg in cell G2 + 2 x Molecular weight of Cl in cell G4
Molecular weight of NaCl in cell B5 = Molecular weight of Na in cell G3 + Molecular weight of Cl in cell G4
Molecular weight of MgO in cell B6 = Molecular weight of Mg in cell G2 + Molecular weight of O in cell G5
The mass of salt in one liter of brine in cell A11 = 1M MgCl2 x Molecular weight of MgCl2 +3.6 M NaCl x molecular weight of NaCl
The mass of water in 77ml of brine in cell B11 = the weight of 77 ml brine- weight of salts in 77 ml of brine =
77 ml x brine density - 77 ml / 1000 ml x (1 M MgCl2 x molcular weight of MgCl2 +3.6 M NaCl x molecular weight of NaCl)
The amount (mole) of MgO in one kg of water in cell F11 = (3.1 g MgO / molecular weight of MgO)/ volume of water in 77 ml of brine x 1000 ml of water / kg water
Molality to molarity conversion factor in cell H11= 77 ml brine/ volume of water in 77 ml of brine

Output
The amount of salts in one liter of brine in Cell A11 is going to be used in EQ3 input file "sgwbb.3i"
The amount (mole) of MgO in one kg of water in Cell F11 is going to be used in EQ6 input file " sgwbb-77.6i"
The molality to molarity conversion factor in cell H11 will be used in Excel file "plots (review)", on worksheet "calculated molality", Cell CF5

		MW	
11ml	1M $MgCl_2$ + 3.6M NaCl	Mg (g/mol)	24.305
3.0 g	MgO	Na (g/mol)	22.989768
$MgCl_2$ (g/mole)	95.2104	Cl (g/mol)	35.4527
NaCl (g/mole)	58.44247	O (g/mol)	15.9994
MgO (g/mole)	38.98917		
Density (simplified GWB)) (g/ml)1	1.1992 (wipp-MgO-CBD-26, p82)		
	Water in 11ml of brine (g)	moles of MgO/kg of water (mol/kg)	
	9.8296	7.8279	

Input

Reaction condition: 3.0g of MgO hydrated in 11ml of simplified GWB (i.e. 1M $MgCl_2$ +3.6 M NaCl)
Simplified GWB density = 1.1992 g/l recorded in WIPP-MgO-CBD-26, p82

Calculation

Molecular weight of $MgCl_2$ in cell B36 = Molecular weight of Mg in cell G34 + 2 x Molecular weight of Cl in cell G37
Molecular weight of NaCl in cell B37 = Molecular weight of Na in cell G35 + Molecular weight of Cl in cell G36
Molecular weight of MgO in cell B38 = Molecular weight of Mg in cell G34 + Molecular weight of O in cell G37
The mass of water in 11 ml of brine in cell B43 = the weight of 11 ml brine - salts in the brine =
11 ml x brine density - 11 ml / 1000 ml x (1M $MgCl_2$ x molcular weigt of $MgCl_2$ + 3.6 M NaCl x molecular weight of NaCl)
The amount (mole) of MgO in one kg of water in cell F43 = (3.0g / molecular weight of MgO) / volume of water in 11 ml of brine x 1000 ml of water / kg water

Output

The amount (mole) of MgO in one kg of water in Cell F43 is going to be used in EQ6 input file " sgwbb-11.6i"

		MW			
77ml	GWB	Mg (g/mol)	24.305	H	1.00794
3.1 g	MgO	Na (g/mol)	22.989768		
		Cl (g/mol)	35.4527		
		O (g/mol)	15.9994		
MgO (g/mole)	38.98917				
Density (GWB) (g/ml)	1.2368				
grams of salt per liter of brine (g/L)	Water in 77 ml of brine (g)	moles of MgO/kg of water (mol/kg)			
348.8832	68.3696	1.1629			

Input	Reaction condition: 3.1g of MgO hydrated in 77ml of GWB (brine recipe = SP 20-4 appendix B) GWB density = 1.2368 g/ml, according to SP 20-4
Calculation	Molecular weight of MgO in cell B6 = Molecular weight of Mg in cell G2 + Molecular weight of O in cell G5 The mass of salt in one liter of brine in cell A11 = (total weight of salt - water in salts Na2B4O710H2O, MgCl2 6H2O and CaCl2 2H2O) / liter of brine (see SP20-4 Appendix A for total weight of salt, Appendix B for concentration of Na2B4O710H2O, MgCl2 6H2O, CaCl2 2H2O) The amount of water in 77 ml of brine in cell B11 = the weight of 77 ml brine- salts in the brine = 77 ml x brine density - 77 ml / 1000 ml x (total weight of salt in 1L of GWB from SP 20-4, appendix A,B) The amount (mole) of MgO in one kg of water in cell F11= (3.1 g MgO / molecular weight of MgO)/ volume of water in 77 ml of brine x 1000 ml of water / kg water
Output	The amount (mole) of MgO in one kg of water in Cell F11 is used in the EQ6 input file " gwb-77.6i"

11 ml	GWB
3.0 g	MgO

MgO (g/mole)	38.98917
Density (GWB) (g/ml)	1.2368

Water in 11ml of brine (g)	MgO mole/kg of water (mol/kg)
9.7671	7.8779

Input

Reaction condition: 3.0g of MgO hydrated in 11ml of GWB
GWB density = 1.2368 g/ml recorded in WIPP-MgO-CBD-26, p82

Calculation

The mass of water in 11 ml of brine in cell B40 = the weight of 11 ml brine- weight of salts in the brine =
11 ml x brine density - 11 ml / 1000 ml x (total weight of salts in SP 20-4 appendix A)
The amount (mole) of MgO in one kg of water in cell F40 = (3.0g / molecular weight of MgO) / volume of water in 11 ml of brine x 1000 ml of water / kg water

Output

The amount (mole) of MgO in one kg of water in Cell F40 is going to be used in EQ6 input file " gwb-11.6i"

77ml	ERDA-6	MW			
3.1 g	MgO	Mg (g/mol)	24.305	H	1.00794
		Na (g/mol)	22.989768		
		Cl (g/mol)	35.4527		
		O (g/mol)	15.9994		
MgO (g/mole)	38.98917				
Density (ERDA) (g/ml)	1.1918				
Salt (g)	Water in 77 ml of brine (g)	moles of MgO/kg of water (mol/kg)			
300.0055	68.6682	1.1579			
		moles of CaO/kg of water (mol/kg)			
		0.007662417			

Input

Reaction condition: 3.1g of MgO hydrated in 77ml of ERDA-6 (brine recipe = SP 20-4 appendix B)
ERDA-6 density = 1.1918 g/ml, according to SP 20-4
The weight ratio of CaO to MgO = 0.63 / 95.2 (see table 8 of Experimental work conducted on MgO characterization and hydration, Deng et al, 2008)

Calculation

Molecular weight of MgO in cell B6 = Molecular weight of Mg in cell G2 + Molecular weight of O in cell G5
The mass of salt in one liter of brine in cell A11 = (total weight of salt - water in salts Na2B4O710H2O, MgCl2 6H2O and CaCl2 2H2O) / liter of brine (see SP20-4 appendix A for total weight of salt, appendix B for concentration of Na2B4O710H2O, MgCl2 6H2O, CaCl2 2H2O)
The amount of water in 77 ml of brine in cell B11 = the weight of 77 ml brine - salts in the brine =
77 ml x brine density - 77 ml / 1000 ml x (total weight of salt in SP20-4 appendix A)
The amount (mole) of MgO in one kg of water in cell F11 = (3.1g / molecular weight of MgO)/ water in 77 ml of brine x 1000 ml of water / kg water
The amount (mole) of CaO in one kg of water in cell F15 = mole of MgO in one kg of water in cell F11 x (0.63/95.2).

Output

The amount (mole) of CaO in one kg of water in cell F15 will be used in EQ6 input file " erdca-77.6i"
The amount (mole) of MgO in one kg of water in Cell F11 is going to be used in EQ6 input file " erdca-78.6i"

11 ml	ERDA-6
3.0 g	MgO

Density(ERDA-6) (g/ml) 1.1918

Water in 11 ml of brine (g)
9.8097

moles of MgO/kg of water (mole/kg)
7.8437

moles of CaO/kg of water (mol/kg)
0.051906699

Input

Reaction condition: 3.0 g of MgO hydrated in 11 ml of ERDA-6 (brine recipe = SP 20-4 appendix B)
ERDA-6 density = 1.1918 g/ml, according to SP 20-4
The ratio of CaO to MgO =0.63 / 95.2 (see table 8 of Experimental work conducted on MgO characterization and hydration, Deng et al, 2008)

Calculation

Molecular weight of MgO in cell B6 = Molecular weight of Mg in cell G2 + Molecular weight of O in cell G5
The amount of water in 11 ml of brine in cell B40 = the weight of 11 ml brine- salts in the brine =
11 ml x brine density - 11 ml / 1000 ml x (total weight of salt in SP20-4 appendix A)
The amount (mole) of MgO in one kg of water in cell F40 = (3.0g / molecular weight of MgO)/ water in 11 ml of brine x 1000 ml of water / kg water
The amount (mole) of CaO in one kg of water in cell F44 = mole of MgO in one kg of water in cell F43 x (0.63/95.2).

Output

The amount (mole) of CaO in one kg of water in cell F40 will be used in EQ6 input file " erdca-11.6i"
The amount (mole) of MgO in one kg of water in Cell F44 is going to be used in EQ6 input file " erdca-12.6i"