Geohydrological Assessment of the proposed the mining activities at Farm RE13/12 Wolvekop, north of Middelburg, Eastern Cape.

REPORT: GEOSS Report No: 2021/06-34 ***PREPARED FOR:*** Ntsanko Ndlovu Group Environmental Specialist Afrimat 012 664 5649 Email: Ntsanko.ndlovu@afrimat.co.za	***PREPARED BY:*** Neville Paxton GEOSS South Africa (Pty) Ltd Unit 12, Technostell Building, 9 Quantum Street, Techno Park Stellenbosch 7600 Tel: (021) 880-1079 Email: info@geoss.co.za (www.geoss.co.za)

GROUNDWATER AND EARTH SCIENCES
GEOSS
SOUTH AFRICA (Pty) Ltd

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EXECUTIVE SUMMARY

Ntsanko Ndlovu of Afrimat appointed GEOSS South Africa (Pty) Ltd to complete a geohydrological assessment to assess potential groundwater impacts associated with a proposed dolerite quarry north of Middelburg, Eastern Cape. This will be an open cast operation where the bench cut method will used to extract sub-base and base gravel aggregates.

The quarrying will entail opening of the surface through open cast mining methods. The applicant will:

- Drill and blast the hard rock after the topsoil of the area has been stripped and stockpiled
- Load and haul the material out of the excavation to the crushing and screening plants
- Crush and screen the recovered material at the crusher plant in order to reduce it to various size aggregate,
- Stockpile the aggregate at a stockpile area until it is collected by clients.

The proposed site has been used for this purpose previously and this will be a re-activation of the quarry activities. A hydrogeological assessment is required to evaluate the potential groundwater impacts of the proposed activities.

The geology underlying the quarry site comprises a massive dolerite intrusion which is surrounded by sandstone and mudstone of the Katberg Formation of the Beaufort Group. Towards the Droë Rivier approximately 1.1 km east of the quarry, alluvial material overlies the Katberg hostrock.

The underlying aquifer at the site is classified by the Department of Water Affairs and Forestry (DWAF, 2002) as a fractured aquifer with an average yield potential of over 5 L/s. This high yield potential was confirmed when finding high yielding boreholes during the hydrocensus approximately 1.7 km away from the Wolvekop Quarry, located in the fractured Katberg Formation and alluvial areas. Based on the DWAF (2002) mapping of the regional groundwater quality, as indicated by electrical conductivity (EC), the area is in the range of 0 – 70 mS/m. This is considered to be "good" quality for water with respect to drinking water standards.

From the desktop study and field work, one active borehole was found within a 1 km radius of the quarry site. This borehole located approximately 300 m away, is low yielding and currently used for stock watering, and is equipped with a windpump. Groundwater use increases towards the Droë Rivier approximately 1.7 km away where high yielding boreholes are drilled into the fractured Katberg Formation.

The aquifer vulnerability to contamination is classified, according to the DRASTIC method, to be "low/medium". This rating is likely associated with the upper intergranular material of the alluvium over 1 km east of the quarry site, and would otherwise be low over the quarry site. DWAF have classified the aquifer below the quarry as being fractured which implies the groundwater is from the fractured bedrock. The bedrock consists of a massive dolerite intrusion which is dense and of low permeability within the location of the quarry site.

The risk associated to groundwater pertains to the operational mining phase only. The operational phase with potential sources relates to nitrates from blasting, leaking of hydrocarbons from machinery and equipment and dust suppression with the quarry water (pit lake water).

Contamination of the fractured aquifer is unlikely to occur due to the low permeability of the massive dolerite. However, it is was seen that the water within the existing and inactive quarry does have elevated concentrations of nitrate, sulphate and sodium, and contamination of natural surface water bodies will occur if the quarry water is disposed in drainage channels.

Given the low to medium vulnerability of the aquifer, together with the above-mentioned factors, **the risk of potential contamination due to the proposed activities to the fractured aquifer is considered to be low**. It will however be important to ensure best management practices are implemented to avoid any unnecessary contamination from occurring.

Recommendations:

From a hydrogeological perspective, activities of the Wolvekop Quarry will have a minimal impact on the groundwater of the area. As the Quarry Water (rainfall held within the excavation) is of poorer quality than the surrounding groundwater, with regards to elevated sodium, nitrates, and sulphates, unnecessary discharge into any proximal drainage channels must be avoided. The water can be used for dust suppression when and if necessary, as the water will evaporate before infiltration into the hard, and low permeable bedrock below the quarry site area.

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TABLE OF CONTENTS

LIST OF MAPS AND FIGURES

LIST OF TABLES

ABBREVIATIONS

BH	Borehole
CGS	Council for Geoscience
DWA	Department of Water Affairs (used to be Department of Water Affairs and Forestry)
DWAF	Department of Water Affairs and Forestry
DWS	Department of Water Affairs and Sanitation
EC	electrical conductivity
L/s	litres per second
m	metres
mbch	meters below collar height
mbgl	metres below ground level
mm	millimetre
mS/m	milli-Siemens per metre
NGA	National Groundwater Archive
WARMS	Water Authorisation and Registration Management System

GLOSSARY OF TERMS

Aquifer: a geological formation, which has structures or textures that hold water or permit appreciable water movement through them [from National Water Act (Act No. 36 of 1998)].

Borehole: includes a well, excavation, or any other artificially constructed or improved groundwater cavity which can be used for the purpose of intercepting, collecting or storing water from an aquifer; observing or collecting data and information on water in an aquifer; or recharging an aquifer [from National Water Act (Act No. 36 of 1998)].

Electrical Conductivity: the ability of groundwater to conduct electrical current, due to the presence of charged ionic species in solution (Freeze and Cherry, 1979).

Fractured aquifer: Fissured and fractured bedrock resulting from decompression and/or tectonic action. Groundwater occurs predominantly within fissures and fractures.

Groundwater: Water found in the subsurface in the saturated zone below the water table or piezometric surface i.e., the water table marks the upper surface of groundwater systems.

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Cover photo:

Photo taken within the quarry showing the stored rainwater.

GEOSS project number:

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Reviewed by:

Julian Conrad (16 July 2021).

1. INTRODUCTION

GEOSS South Africa (Pty) Ltd was appointed by Ntsanko Ndlovu of Afrimat to complete a geohydrological assessment to assess potential groundwater impacts associated with a proposed dolerite quarry north of Middelburg, Eastern Cape. The project entails mining for dolerite best suited for aggregates such as sub-base and base gravel. These will be open cast operations where quarrying will take place through utilising a bench cut method.

The quarrying will entail opening of the surface through open cast mining methods. The applicant will:

- Drill and blast the hard rock after the topsoil of the area has been stripped and stockpiled
- Load and haul the material out of the excavation to the crushing and screening plants
- Crush and screen the recovered material at the crusher plant in order to reduce it to various size aggregate,
- Stockpile the aggregate at a stockpile area until it is collected by clients.

The proposed site has been used for this purpose previously and this will be a re-activation of the quarry activities. A hydrogeological assessment is required to evaluate the potential groundwater impacts of the proposed activities. The quarry is located 13 km north of Middelburg just to the west of the N9 road (**Map 1**).

2. SCOPE OF WORKS

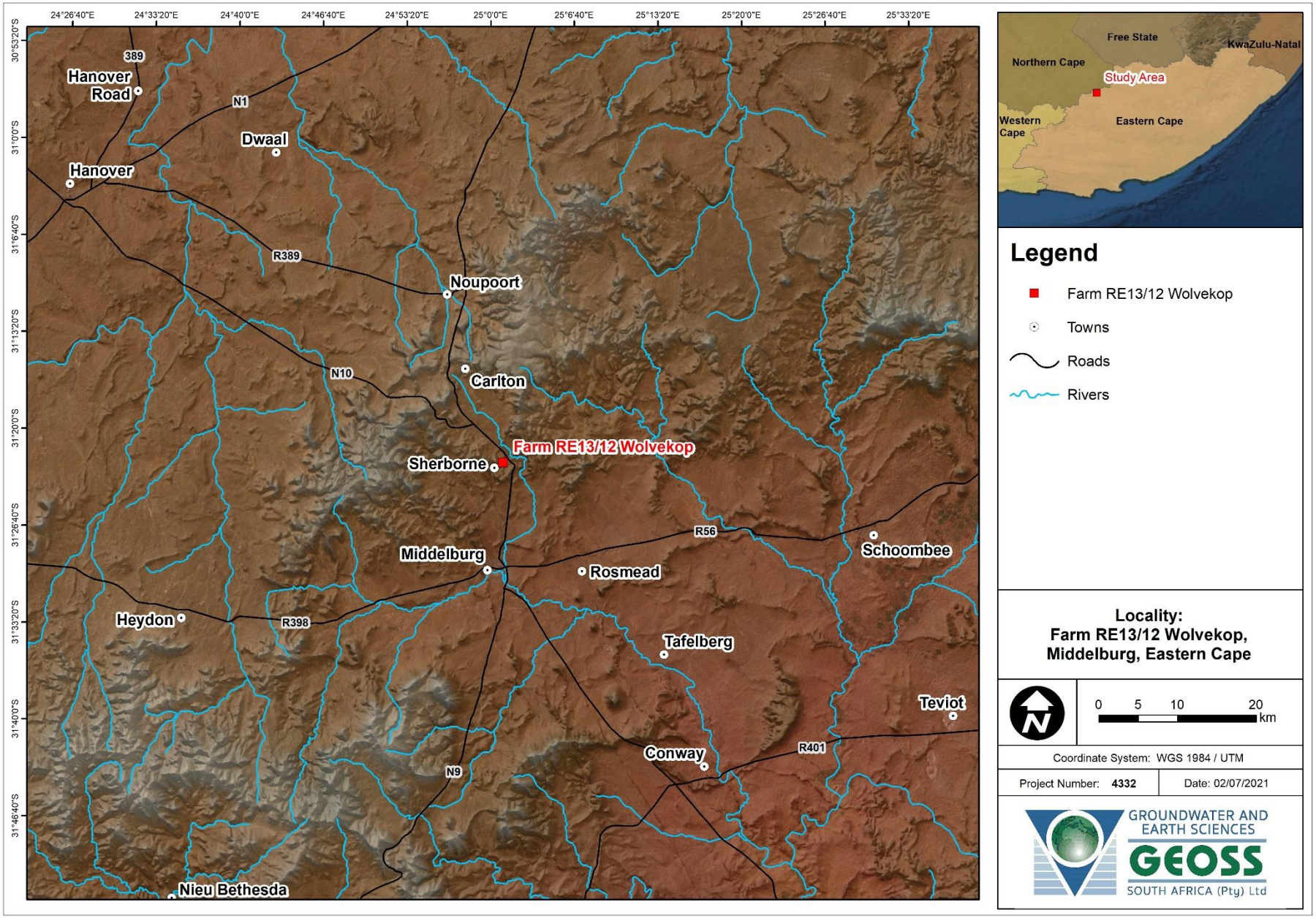
The scope of work is to provide groundwater specialist services, including the tasks outlined below:

- Relevant data will be sourced from the National Groundwater Archive; national scale geological and groundwater maps and consultant reports. A project GIS will be developed. Review of proposed site activities and their potential impacts will be assessed.
- A site visit and hydrocensus will be completed, which will include geological mapping; a hydrocensus and sampling of boreholes within 1 km of the site. During this visit the pollution potential of the activities will be assessed. Provision is made for the collection and submission of up to two groundwater samples to an accredited laboratory for comprehensive SANS241 inorganic analysis.
- The data will be analysed and assessed, and a conceptual site model developed. Groundwater depth and flow direction will be assessed, as well as the potential for inflow into the excavation. Water quality will be assessed, including basic geochemical modelling where required/relevant using the software PHREEQE-C (a programme for geochemical calculations). The results will then be documented in a report presenting the findings as well as relevant recommendations.

3. METHODOLOGY

The procedure adopted for this study involved a desktop study followed by the field work. The desktop study involved obtaining and reviewing relevant data to the project. This included analysing data from the NGA, groundwater yield, groundwater chemistry and geological maps of the area.

A site visit was then conducted to collect additional data and verify as much of the existing data as possible. This included a hydrocensus of groundwater users in the area and noting any subsurface conditions where possible. The site walkover was conducted at the existing inactive quarry. All collected data was analysed and interpreted to assess the potential risks associated with the intended site development as they pertain to groundwater.



Map 1: Locality of the Wolvekop Quarry, Middelburg, Eastern Cape.

4. SETTING

4.1 Topography

The study site is situated in the Eastern Cape in the Middelburg area. The study area slopes gently towards the north east, towards the Droë Rivier. with an average elevation of 1435 m above mean sea level (mamsl). The site is situated in the quaternary catchment, Q14B, which has a General Authorisation abstraction volume of 0 m^3/ha/yr.

4.2 Climate

The study area experiences a summer rainfall climate with cold dry winters. **Figure 1** shows the monthly average air temperature (minimum and maximums) and **Figure 2** shows the monthly median rainfall and days of rainfall per month (worldweatheronline.com). The study area receives a mean annual precipitation average of 320 mm/a.

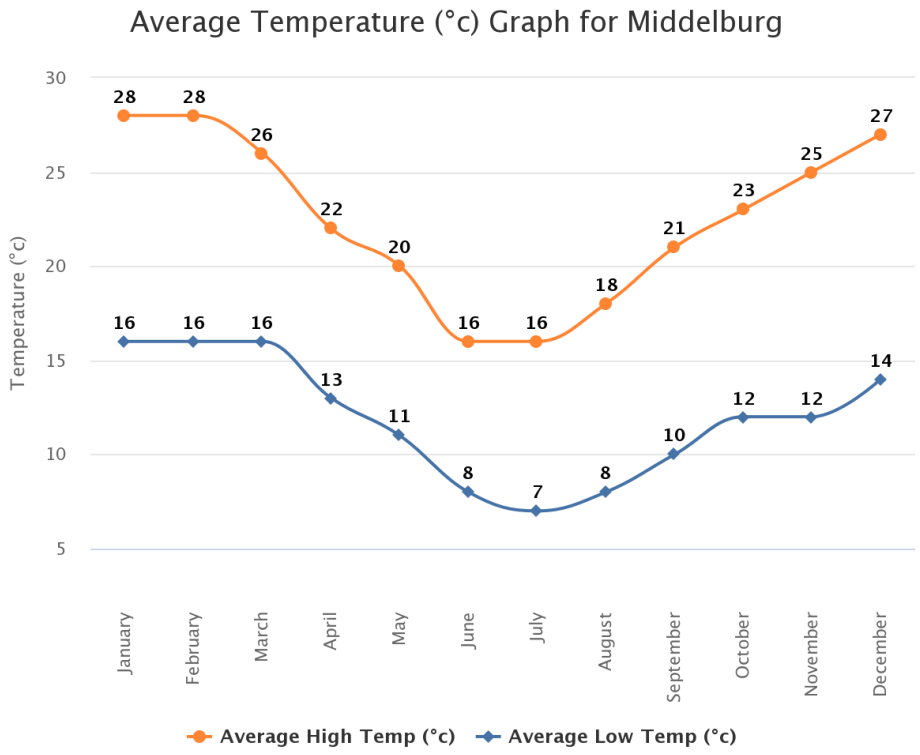


Figure 1: Monthly average air temperature for the study area (https://www.worldweatheronline.com/).

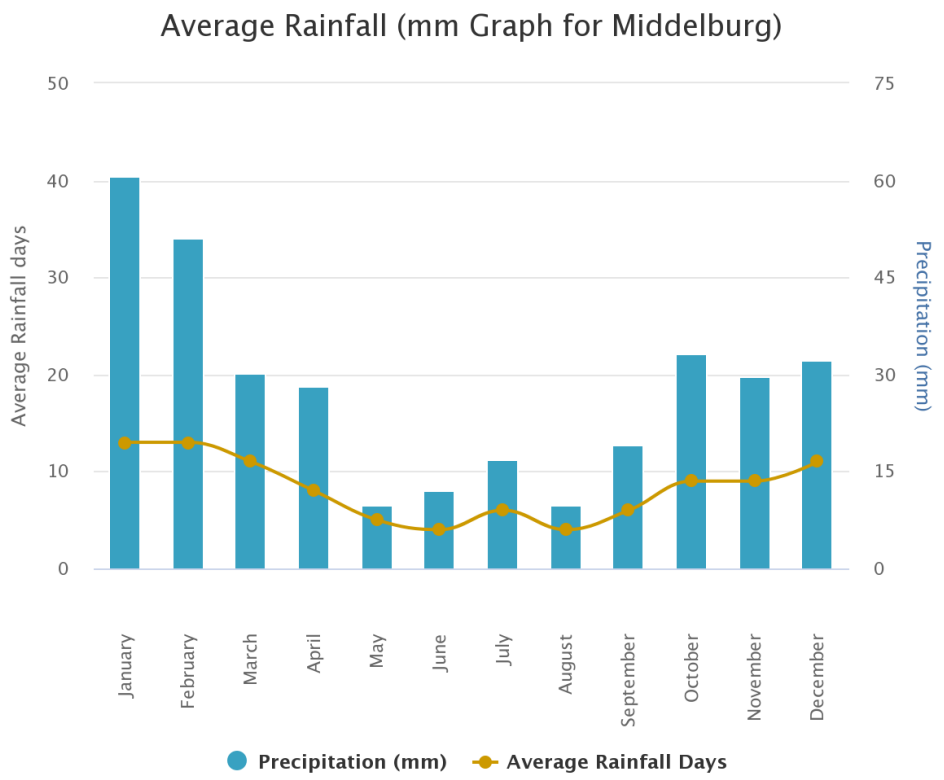


Figure 2: Monthly average rainfall and rainfall distribution for the study area (https://www.worldweatheronline.com/).

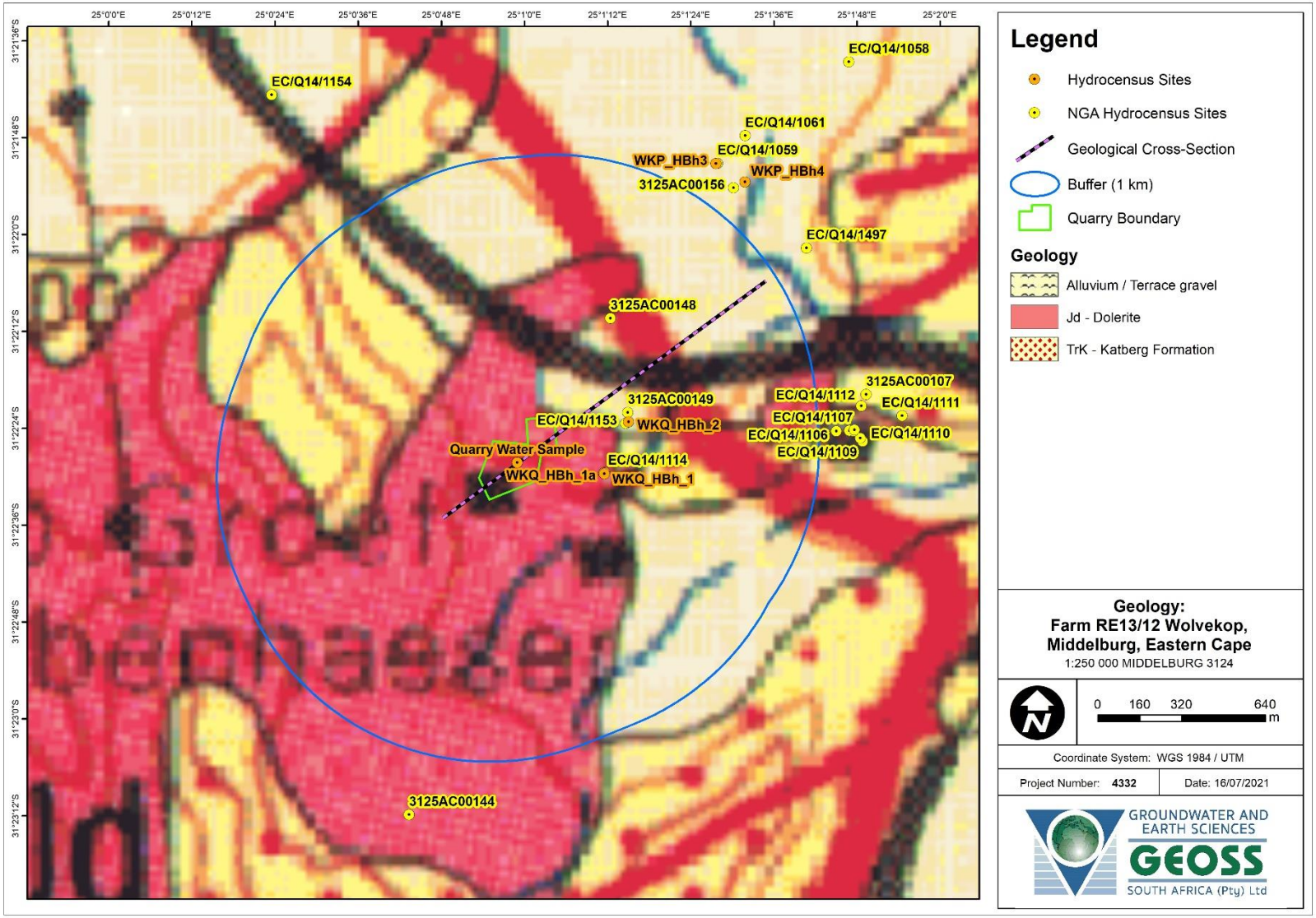
4.3 Geology

The Geological Survey of South Africa (now the Council for Geoscience (CGS)) has mapped the area at 1:125 000 scale (3124 Middelburg). The geological setting is shown in **Map 2** and the main geology of the area is listed in **Table 1**.

Table 1: Geological formations within the study area.

Code	Formation	Group	Description
⌒	Quaternary deposits		Alluvium and terrace gravel
Jd	Intrusive		Dolerite
TrK	Katberg	Beaufort	Sandstone rich with red brown mudstone.

The geology underlying the quarry site comprise a massive dolerite intrusion which is surrounded by sandstone and mudstone of the Katberg Fromation of the Beaufort Group. Towards the Droë Rivier alluvial material overlies the Katberg hostrock. A simple geological conceptual model is presented in **Figure 3**.



Map 2: Geological setting of the study area and surrounds, (1:125 000 scale 3124 Middelburg (CGS, ~1975)).

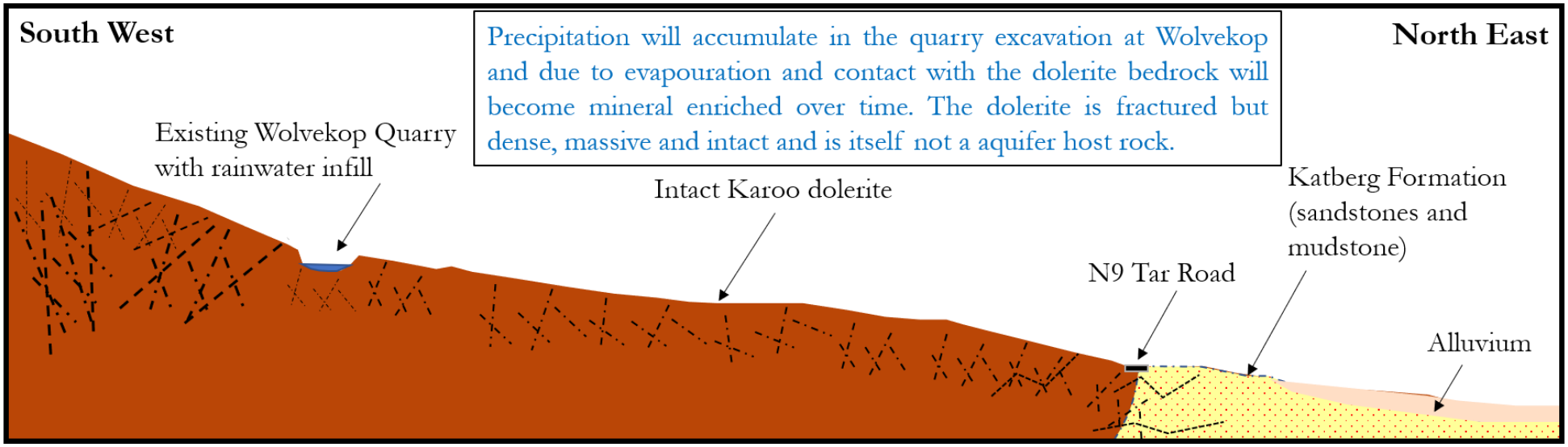


Figure 3: Conceptual south-west / north-east geological cross-section.

4.1 Hydrogeology

The underlying aquifer at the site is classified by the Department of Water Affairs and Forestry (DWAF, 2002) as a **fractured aquifer** with an average **yield potential of over.5 L/s** (**Map 3**). This high yield potential was confirmed when finding high yielding boreholes during the hydrocensus which were located in the fractured Katberg Formation and alluvial areas – well away from the Wolvekop Quarry. A fractured aquifer describes an aquifer where groundwater occurs in narrow fractures within the bedrock. Based on the DWAF (2002) mapping of the regional **groundwater quality**, as indicated by electrical conductivity (EC), the area is in the range of 0 – 70 mS/m. This is considered to be "**good**" quality for water (**Map 4**), with respect to drinking water standards.

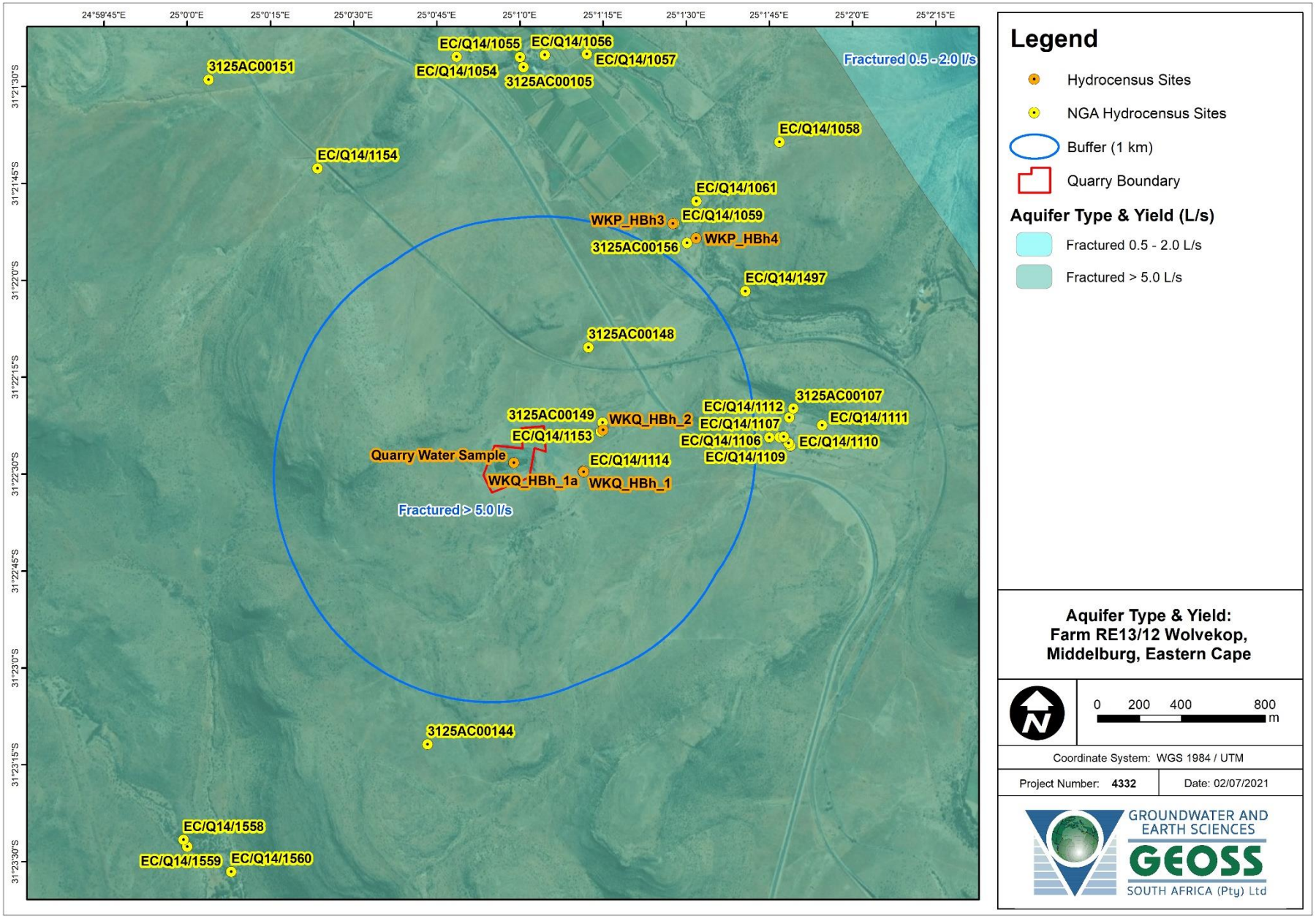
4.2 Aquifer vulnerability classification

The national scale groundwater vulnerability map, which was developed according to the DRASTIC methodology (Conrad and Munch, 2007), indicates that the site has a "**low/medium**" **vulnerability** to surface-based contaminants (**Map 5**).

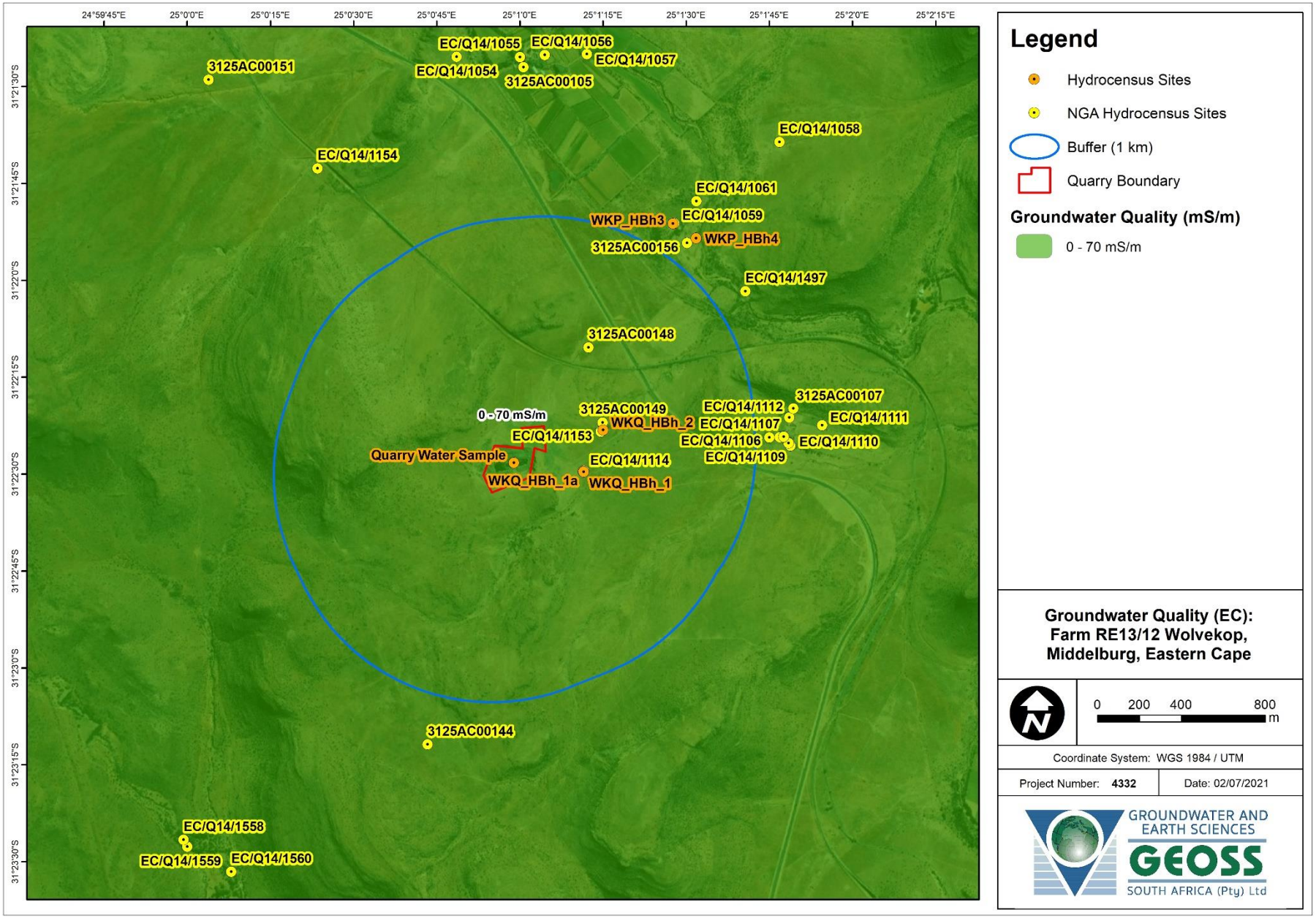
The DRASTIC method considers the following factors:

D = depth to groundwater (5);
R = recharge (4);
A = aquifer media (3);
S = soil type (2);
T = topography (1);
I = impact of the vadose zone (5); and
C = conductivity (hydraulic) (3)

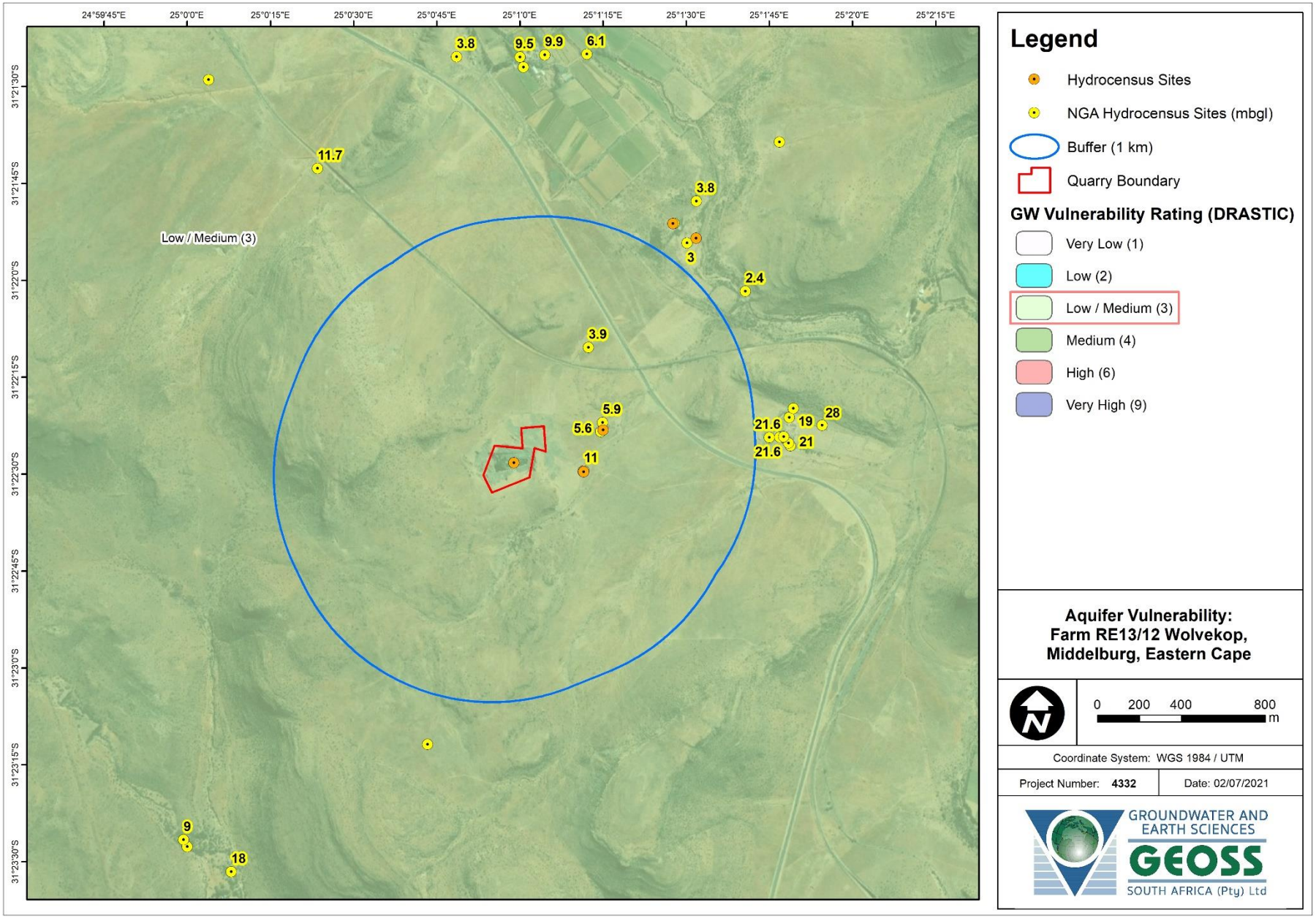
The number indicated in parenthesis at the end of each factor description is the weighting or relative importance of that factor. This "**low/medium**" rating is likely associated with the upper intergranular/alluvial material which is slightly susceptible to point and non-point sources of contamination which occurs closer to the river. There is no alluvial material at the quarry site. DWAF have classified the aquifer as being fractured which implies the groundwater is mainly found in the fractured bedrock below.



Map 3: Regional aquifer yield type (DWAF, 2002) and average borehole yield classification (excluding dry boreholes).



Map 4: Regional groundwater quality (mS/m) from DWAF (2002).



Map 5: Vulnerability rating (DWAF, 2005) and groundwater depths (mbgl).

5. DESKTOP ASSESSMENT AND HYDROCENSUS

5.1 Desktop Assessment

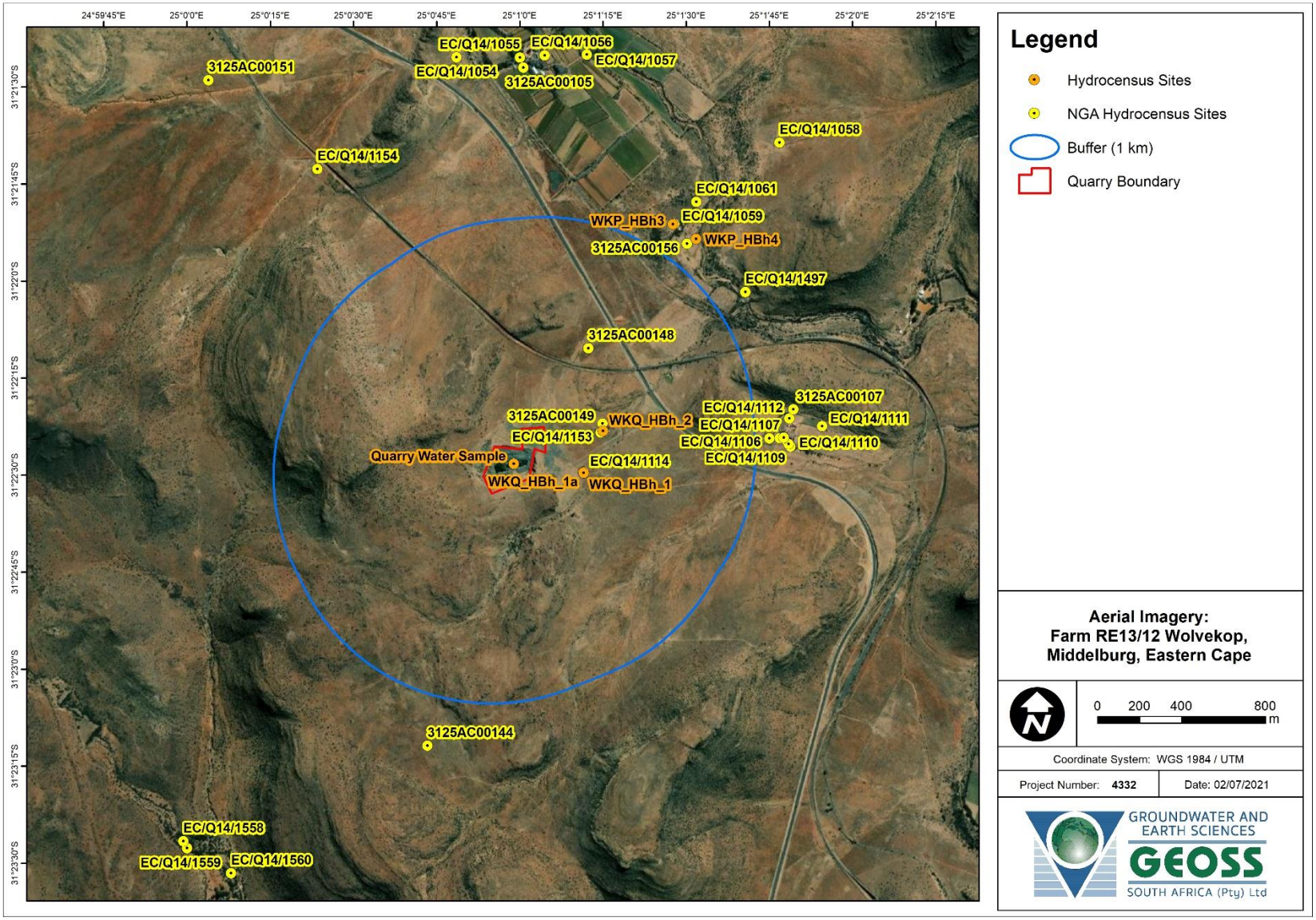
A desktop assessment was initially carried out around the property to determine if there were any groundwater users in the area. The National Groundwater Archive (NGA) database provides data on borehole positions, groundwater chemistry and yield. The NGA indicated that there are 20 boreholes located within the 3 km search area of the site. Those NGA sites that were within the 1 km radius of the site were assessed in the field and further details are presented in the sections below. The NGA borehole details within the 3 km radius are indicated in Map 6 and summarised in **Table 2**.

Table 2: Summary of NGA borehole details.

NGA Identifier	Latitude	Longitude	Water Level (mbgl)	EC (mS/m)
EC/Q14/1560	-31.3921	25.00221	18	-
EC/Q14/1558	-31.39073	24.99982	9	-
EC/Q14/1114	-31.37486	25.01989	11	-
EC/Q14/1110	-31.37378	25.03024	21	-
EC/Q14/1109	-31.37367	25.03014	19.16	-
EC/Q14/1107	-31.37341	25.0297	21.64	-
EC/Q14/1108	-31.37339	25.02991	21.61	61.9
EC/Q14/1153	-31.37317	25.02073	5.56	-
EC/Q14/1111	-31.3729	25.03182	28	-
3125AC00149	-31.37279	25.02082	5.97	-
EC/Q14/1112	-31.37256	25.03018	19	-
3125AC00148	-31.36955	25.02012	3.85	-
EC/Q14/1497	-31.36713	25.02798	2.44	-
3125AC00156	-31.36506	25.02506	3	-
EC/Q14/1061	-31.36326	25.02552	3.8	-
EC/Q14/1154	-31.36186	25.00653	11.65	-
EC/Q14/1055	-31.35707	25.01668	9.5	-
EC/Q14/1054	-31.35705	25.0135	3.8	-
EC/Q14/1056	-31.35698	25.01792	9.86	-
EC/Q14/1057	-31.35694	25.02003	6.07	-

5.2 Hydrocensus

A site visit was carried out on 4 June 2021 to assess groundwater use within the study area Three groundwater sources could be identified. These sites are summarised in **Table 3** and together with NGA sites are presented in **Map 6**. Based on the data it is evident that there are a number of groundwater users surrounding the proposed development, however, information on these boreholes is somewhat limited. From the data, water levels vary across the area, but tend to follow the topographic trend with the deepest levels higher up and the shallowest levels closer to the Droë Rivier. Water samples were collected from the closest active borehole to the site (WKQ_HBh2) and the quarry itself (Quarry_Water), the positions for which are presented in **Map 7**.



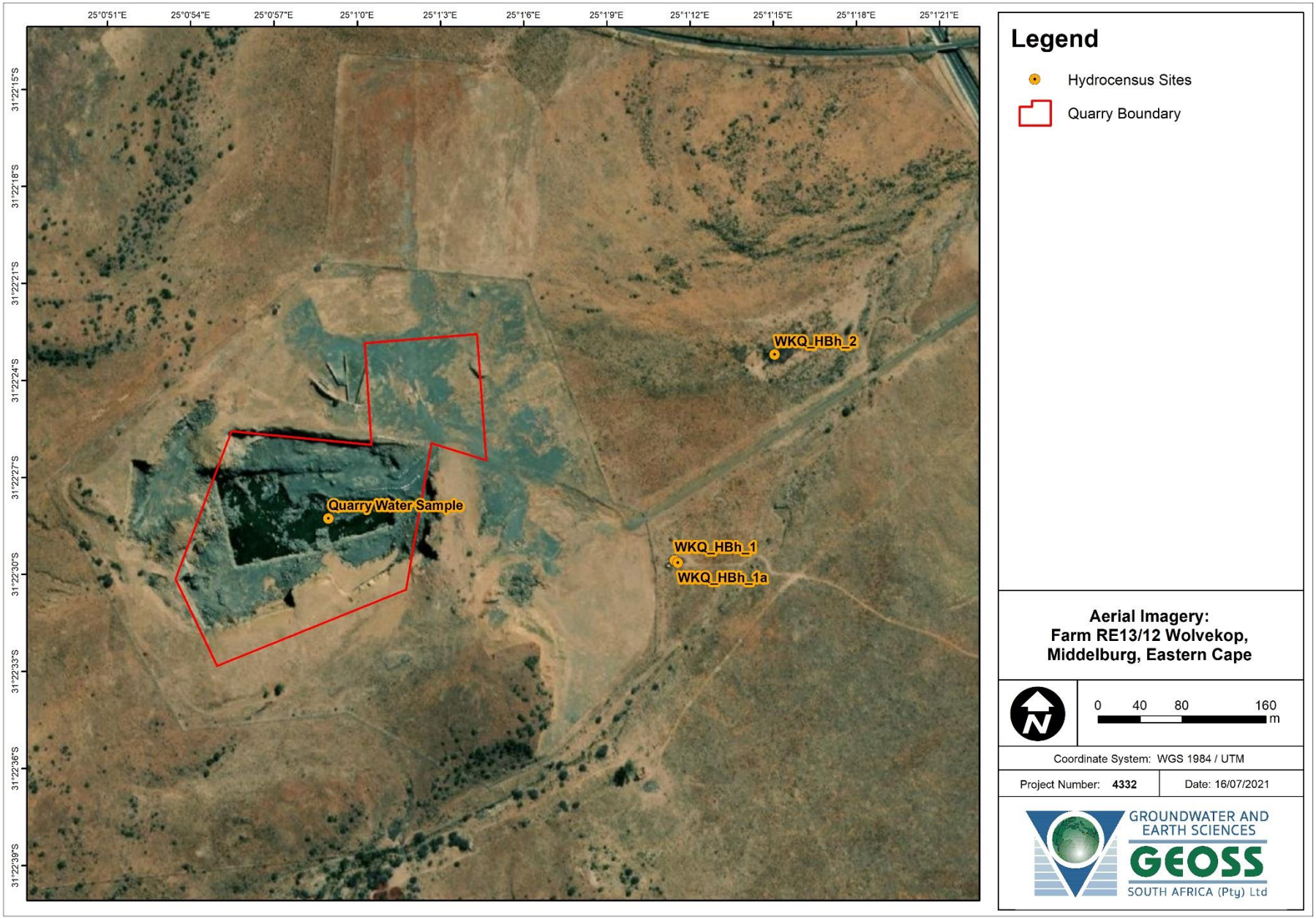
Map 6: Study site with 1 km buffer area including NGA positions both within and outside of the1 km buffer area.

Table 3: Hydrocensus details from the site visit.

Hydrocensus Point	NGA Identifier	Latitude	Longitude	Water Level (mbgl)	Comments	Photo
Quarry Water Sample	n/a	-31.374520°	25.016380°	Not applic-able	Definite layering of precipitate at the varying water level marks (See photo). Precipitate sour to the taste, possibly gypsum. Notable algal growth layer on bottom of quarry, indicating long standing water. Very clear water (100% visibility).	
WKQ_HBh_1	EC/Q14/1114	-31.374880°	25.019850°	Dry	Windpump in good condition, but tail tied down (not operating) Dam empty.	

WKQ_HBh_1a	EC/Q14/1114	-31.374900°	25.019880°	Dry	Dry/collapsed at 7.5 mbgl	
WKQ_HBh_2	EC/Q14/1153	-31.373110°	25.020850°	~13.5	Blocked dipmeter at 8.5 mbgl - no water yet. Sampled for laboratory analysis. Windpump also tied down but working. Farmer (Johan Appelgrein) says there are 6 to 7 pipes, with one below water table. Therefore, water level ~ 13.5 mbgl.	

WKP_HBh3	EC/Q14/1059	-31.364220°	25.024350°	Unable to access	Pumped up to 80 m3/hour during the day only. Used as a backup only. Not able to get water level. Borehole is equipped with a mono-pump and sealed at the top.	
WKP_HBh4	3125AC00156	-31.364850°	25.025510°	Unable to access on site visit. 3 m (NGA record)	Unable to access water level.	
-	3125AC00148	-31.369550°	25.020120°	Not found in field3.85 (NGA record)	Not found in field.	



Map 7: Aerial image with hydrocensus boreholes and sampling sites.

5.3 Groundwater flow direction

Groundwater level data was obtained from the NGA database, in an effort to determine flow direction. The data together with field data was used to generate a groundwater level contour map to determine groundwater flow direction. **Map 8** shows the general flow direction across the study area. The groundwater locally flows southwest towards the Droë Rivier drainage channel where after it flows south parallel to the N9 Road.

In order to evaluate the relationship between groundwater levels and topography, and the applicability of the interpolation technique, the surface elevations and water table elevations are plotted relative to each other. The data is presented in **Figure 4**, and indicates a 69% correlation between surface topography and water level elevation. Bayesian interpolation is therefore a good guide for establishing water flow direction, though in field measurements and kriging based on topography was used to generate the map for a higher degree of confidence.

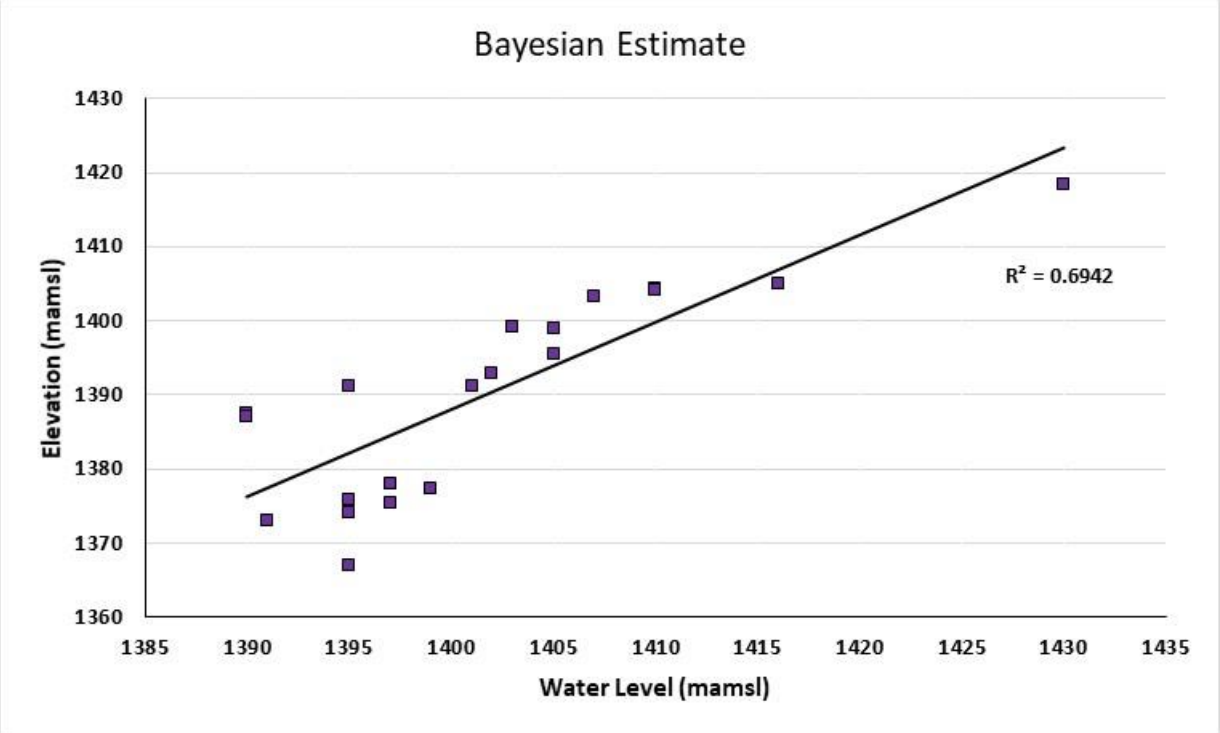
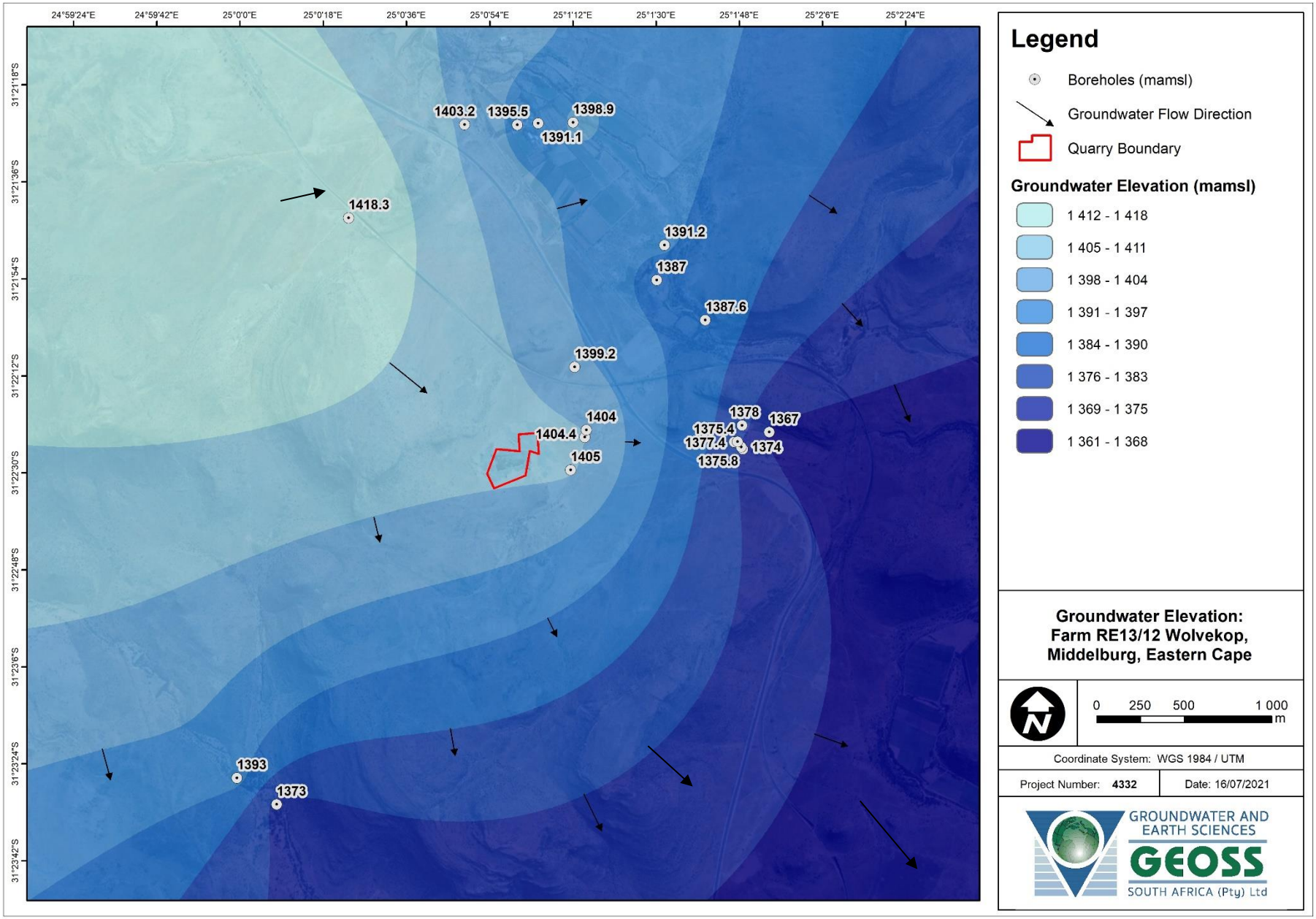


Figure 4: Correlation between surface topography and groundwater elevation for boreholes proximal to study site.



Map 8: Groundwater elevation (mamsl) map showing boreholes and flow directions.

5.4 Water Quality Analysis

Two water samples, namely Quarry_Water (sample taken from standing water in quarry) and WKQ_HBh2 (nearest active borehole to quarry) were collected during the site visit and submitted for inorganic chemical analysis to a SANAS accredited laboratory (Vinlab) in the Western Cape. The certificate of analysis for all the samples is presented in **Appendix A**.

The chemistry results were classified according to the SANS241-1: 2015 standards for domestic water. **Table 4** enables an evaluation of the water quality with regards to the various limits, colour coded according to the SANS241-1: 2015 drinking water assessment standards.

Table 4: Classification table for specific limits

Acute Health	**Aesthetic**	**Chronic Health**	**Operational**	**Acceptable**

Analyses	WKQ_HBh2	Quarry Water	SANS 241-1:2015
pH (at 25 °C)	7.4	8.2	≥5 - ≤9.7 Operational
Conductivity (mS/m) (at 25 °C)	76.8	298.0	≤170 Aesthetic
Total Dissolved Solids (mg/L)	520.70	2020.44	≤1200 Aesthetic
Turbidity (NTU)	2.10	1.20	≤5 Aesthetic ≤1 Operational
Colour (mg/L as Pt)	<15	<15	≤15 Aesthetic
Sodium (mg/L as Na)	23	532	≤200 Aesthetic
Potassium (mg/L as K)	1	4	N/A
Magnesium (mg/L as Mg)	39	9	N/A
Calcium (mg/L as Ca)	71	124	N/A
Chloride (mg/L as Cl)	19.99	72.88	≤300 Aesthetic
Sulphate (mg/L as SO_4)	63.01	1220.08	≤250 Aesthetic ≤500 Acute Health
Nitrate Nitrogen (mg/L as N)	5.08	57.84	≤11 Acute Health
Nitrite Nitrogen (mg/L as N)	<0.05	0.06	≤0.9 Acute Health
Ammonia Nitrogen (mg/L as N)	<0.15	<0.15	≤1.5 Aesthetic
Total Alkalinity (mg/L as $CaCO_3$)	312.4	62.5	N/A
Total Hardness (mg/L as $CaCO_3$)	337.4	346.9	N/A
Fluoride (mg/L as F)	0.43	0.51	≤1.5 Chronic Health
Aluminium (mg/L as Al)	0.011	0.028	≤0.3 Operational
Total Chromium (mg/L as Cr)	<0.004	<0.004	≤0.05 Chronic Health
Manganese (mg/L as Mn)	0.005	<0.018	≤0.1 Aesthetic ≤0.4 Chronic Health
Iron (mg/L as Fe)	0.244	0.012	≤0.3 Aesthetic ≤2 Chronic Health
Nickel (mg/L as Ni)	<0.008	<0.008	≤0.07 Chronic Health
Copper (mg/L as Cu)	0.024	0.013	≤2 Chronic Health
Zinc (mg/L as Zn)	0.040	<0.008	≤5 Aesthetic
Arsenic (mg/L as As)	<0.010	0.051	≤0.01 Chronic Health
Selenium (mg/L as Se)	<0.008	<0.008	≤0.04 Chronic Health
Cadmium (mg/L as Cd)	0.001	0.001	≤0.003 Chronic Health
Antimony (mg/L as Sb)	<0.013	0.016	≤0.02 Chronic Health
Mercury (mg/L as Hg)	<0.001	<0.001	≤0.006 Chronic Health
Lead (mg/L as Pb)	<0.008	0.008	≤0.01 Chronic Health
Uranium (mg/L as U)	<0.028	<0.028	≤0.03 Chronic Health
Cyanide (mg/L as CN^-)	<0.01	<0.01	≤0.2 Acute Health
Total Organic Carbon (mg/L as C)	1.06	2.06	N/A
Charge balance %	-2.1	2.4	≥-5 - ≤5 Acceptable

The chemistry results obtained were also classified according to the DWAF (1998) standards for domestic water. **Table 5** enables an evaluation of the water quality with regards to the various parameters measured (DWAF, 1998). **Table 6** presents the water chemistry analysis results colour coded according to the DWAF drinking water assessment standards.

Table 5: Classification table for the groundwater results (DWAF, 1998)

Blue	**(Class 0)**	**Ideal water quality** - suitable for lifetime use.
Green	**(Class I)**	**Good water quality** - suitable for use, rare instances of negative effects.
Yellow	**(Class II)**	**Marginal water quality** - conditionally acceptable. Negative effects may occur.
Red	**(Class III)**	**Poor water quality** - unsuitable for use without treatment. Chronic effects may occur.
Purple	**(Class IV)**	**Dangerous water quality** - totally unsuitable for use. Acute effects may occur.

Table 6: Classified groundwater sample results according to DWAF 1998.

Sample Marked :	**WKQ_HBh2**	**Quarry Water**	**DWA (1998) Drinking Water Assessment Guide**				
			Class 0	**Class I**	**Class II**	**Class III**	**Class IV**
pH	7.4	8.2	5-9.5	4.5-5 & 9.5-10	4-4.5 & 10-10.5	3-4 & 10.5-11	< 3 & >11
Conductivity (mS/m)	76.8	298.0	<70	70-150	150-370	370-520	>520
Turbidity (NTU)	2.10	1.20	<0.1	0.1-1	1.0-20	20-50	>50
	mg/L						
Total Dissolved Solids	520.70	2020.44	<450	450-1000	1000-2400	2400-3400	>3400
Sodium (as Na)	23	532	<100	100-200	200-400	400-1000	>1000
Potassium (as K)	1	4	<25	25-50	50-100	100-500	>500
Magnesium (as Mg)	39	9	<70	70-100	100-200	200-400	>400
Calcium (as Ca)	71	124	<80	80-150	150-300	>300	
Chloride (as Cl)	19.99	72.88	<100	100-200	200-600	600-1200	>1200
Sulphate (as SO_4)	63.01	1220.08	<200	200-400	400-600	600-1000	>1000
Nitrate& Nitrite (as N)	5.08	57.90	<6	6.0-10	10.0-20	20-40	>40
Fluoride (as F)	0.43	0.51	<0.7	0.7-1.0	1.0-1.5	1.5-3.5	>3.5
Manganese (as Mn)	0.005	<0.018	<0.1	0.1-0.4	0.4-4	4.0-10.0	>10
Iron (as Fe)	0.244	0.012	<0.5	0.5-1.0	1.0-5.0	5.0-10.0	>10
Copper (as Cu)	0.024	0.013	<1	1-1.3	1.3-2	2.0-15	>15
Zinc (as Zn)	0.040	<0.008	<20	>20			
Arsenic (as As)	<0.010	0.051	<0.010	0.01-0.05	0.05-0.2	0.2-2.0	>2.0
Cadmium (as Cd)	0.001	0.001	<0.003	0.003-0.005	0.005-0.020	0.020-0.050	>0.050
Hardness (as $CaCO_3$)	337.400	346.90	<200	200-300	300-600	>600	
Charge Balance %	-2.1	2.4	≥-5 - ≤5 Acceptable				

From the chemical results presented in **Table 4** and **Table 6**, the groundwater from WKQ_BH2 considered a Class II type water due to Turbidity and Hardness, the latter of which is typical for the formations that host the groundwater. The electrical conductivity of WKQ_BH2 is 76.8 mS/m which is considered good, and within range of the groundwater of the area. The water in the quarry (Quarry_Water) is considered to be Class IV type water due to its elevated sodium, high sulphates, nitrates and nitrites These parameters were within Class 0 (low concentrations) for the groundwater from WKQ_BH2. The EC of the quarry water is also about four times higher than the average salinity of groundwater for the area with a lab measurement of 298 mS/m.

A number of chemical diagrams have been plotted for the water samples and these are useful for chemical characterisation and comparison of the water. The chemistry of the samples has been plotted on a tri-linear diagram known as a Piper diagram. This diagram indicates the distribution of cations and anions in separate triangles and then a combination of the chemistry in the central diamond. From **Figure 5** (central diamond) the water sample collected from the quarry is classified as a sodium–sulphate type water and the groundwater sample (WKQ_HBh2) is classified as a calcium-bicarbonate type water. When plotting to the central right portion of the diamond, a water is considered to be shallow, freshly recharged groundwater. When a sample plots to the right corner of the central diamond the sample may be considered of marine origin, or more relevant here, highly evaporated water.

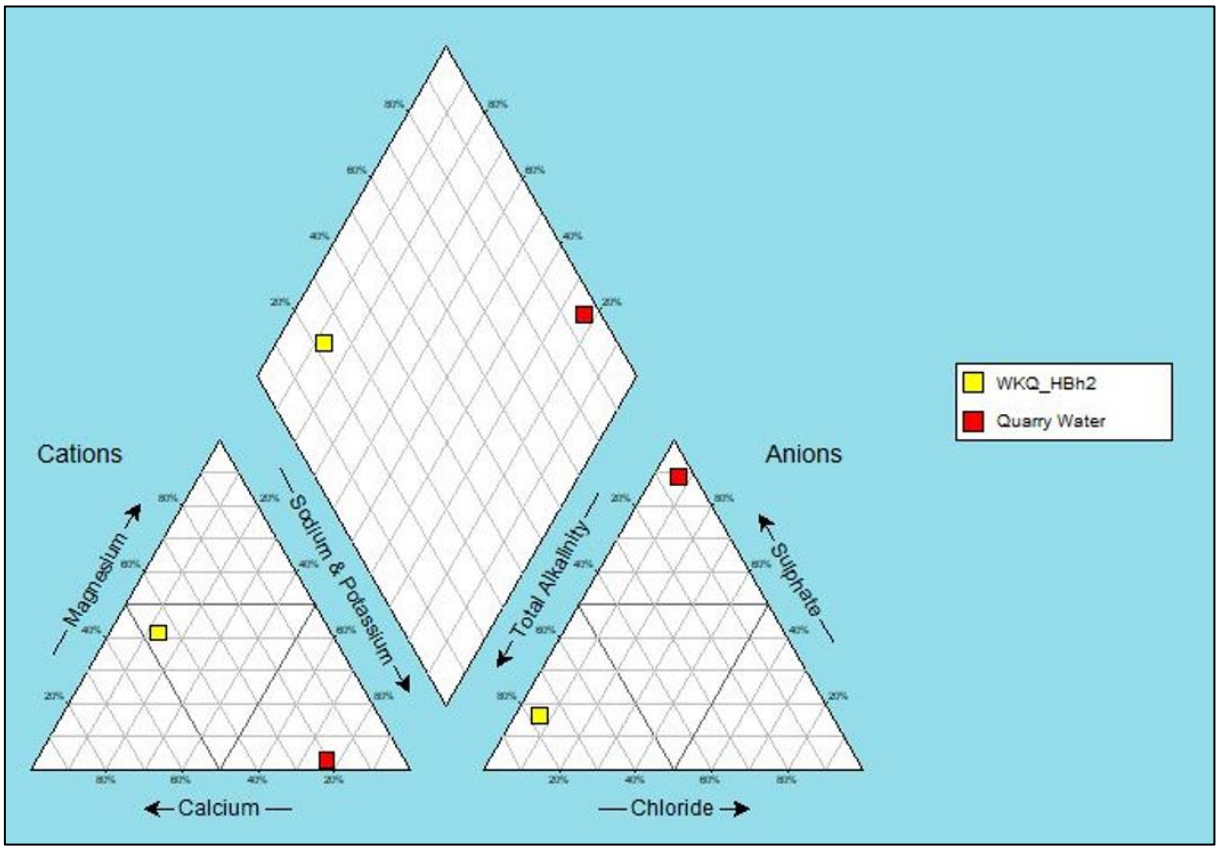


Figure 5: Piper diagram of the groundwater samples.

The Stiff diagram is a graphical representation of the relative concentrations of the cations (positive ions) and anions (negative ions). This diagram shows concentrations of cations and anions relative to each other (not as a percentage as with Piper) and direct reference can be made to specific salts in the water. The Stiff diagram for the samples from the production boreholes are shown in **Figure** 6. From the shape of the Stiff diagram the major ions present in the water can be compared. It is clear that the quarry sample is dominated by Na and SO4 and has a higher dissolved mineral concentration compared to the groundwater sample dominated by Ca and HCO3.

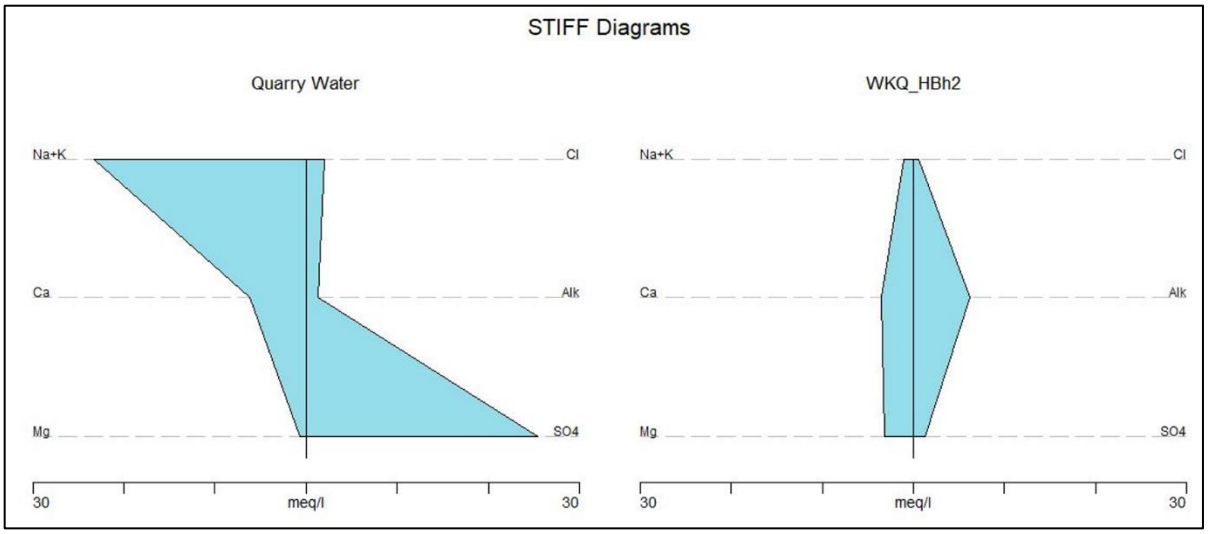


Figure 6: Stiff diagram of the groundwater sample.

5.5 Geochemical Modelling

Geochemical modelling was completed using PHREEQC (llnl database) to gain a better understanding of the groundwater hydrogeochemistry. The first component focussed on the water samples collected on site to determine the geochemical character (water type, chemical species distribution and mineral saturation index). The second component focussed on the impact of local geology on groundwater chemistry.

Two water samples (from quarry and from nearby existing borehole) were collected and submitted for inorganic chemical analysis. The chemistry results were used to run a geochemical model. A summary of the model output is shown in **Table 7** below. The PHREEQC generated data is provided in **Appendix B**.

Table 7: Geochemical modelling result output summary

	Quarry Water	**WKQ_HBh2**
pH (at 25 °C)	8.16	7.36
EC in mS/m (at 25 °C)	298	76.8
Electro neutrality (%)	3.9	2.2
Ionic strength (mol/kg)	4.213e-02 (0.042)	1.140e-02 (0.011)
Water type	Sodium–Sulphate	Calcium-Bicarbonate
Species distribution	HCO_{3-}	HCO_{3-}

(dominant species)	Ca^{2+} Cl^{-} F^{-} Fe^{2+} $Fe(OH)_3$ K^{+} Mg^{+2} NO_{2-} NO_{3-} Na^{+} SO_4^{-2}	Ca^{2+} Cl^{-} F^{-} Fe^{2+} $Fe(OH)_3$ K^{+} Mg^{+2} NO_{2-} NO_{3-} Na+ SO_4^{-2}
Saturation index (Minerals of interest)	Calcite: 0.36 Gypsum: -0.71	Calcite: 0.3 Gypsum: -1.92

The water sample collected from the quarry is characterized as being slightly alkaline pH (8.16) with a moderate dissolved mineral concentration (EC: 298 mS/m). The groundwater sample (WKQ_HBh2) is characterized as having a neutral pH (7.36) with a low dissolved mineral concentration (EC: 76.8 mS/m).

Mineral saturation index is an index that indicates whether a water will tend to dissolve or precipitate a particular mineral. Its value is negative when the mineral may be dissolved, positive when it may be precipitated, and zero when the water and mineral are at chemical equilibrium. The saturation index (SI) is calculated by comparing the chemical activities of the dissolved ions of the mineral (ion activity product, IAP) with their solubility product (Ksp). In equation form, SI = log(IAP/Ksp). Both water samples show a slightly positive SI for Calcite (tend to precipitate) and a negative SI for Gypsum (tend to dissolve).

The second component focussed on the impact of site geological conditions on groundwater chemistry. The geological host rock in the area is dolerite (Karoo Dolerite Suite). No bulk rock chemical/mineralogical results were available from the quarry at the time of this study. Literature chemical and mineralogical data for dolerite was used to run a geochemical model.

The typical mineralogical composition of dolerite is listed below (in order of decreasing composition percentage):

- Plagioclase feldspar (Albite & Anorthite)
- Pyroxenes (usually augite)
- Amphiboles (hornblende)
- Olivine (Fayalite & Forsterite)
- Magnetite
- Quartz

Typical chemical composition (from literature) of dolerite shown in **Table 8** below.

Table 8: Chemical composition of four Karoo Dolerite Suite sills (Marsh et al., 1984)

	Blaauwkranz	**Hangnest**	**Tandjiesberg**	**Amherst**
Mineral	%			
SiO_2	51.25	53.88	51.33	51.73
TiO_2	0.86	1.09	0.9	0.98
Al_2O_3	15.62	15.83	15.96	15.06
Fe_2O_3	10.75	9.96	11.22	11.25
MnO	0.16	0.16	0.17	0.23
MgO	7.58	6.53	6.51	6.92
CaO	10.79	9.24	10.97	10.56
Na_2O	2.31	2.19	2.32	2.49
K_2O	0.54	0.89	0.6	0.61
P_2O_5	0.13	0.22	0.14	0.17
ppm				
Zr	76	150	90	93
Nb	3.8	4.6		4.7
Y	22	26	22	27
Rb	9	21	12	12
Ba	152	310	184	202
Sr	185	201	201	227
Co	53	39	47	50
Ni	107	3.7	70	89
Cr	384	385	265	303
V	232	186	219	235
Zn	76	88	76	86
Cu	96	20	95	81

The first step was to react (equilibrate) pure rainwater with atmospheric CO2 and O2. Secondly running an equilibrium reaction between rainwater and dolerite to simulate a theoretical groundwater hydrochemical composition. The results indicate slightly alkaline pH (~9) with low Ionic strength 3.406e-03 mol/kgw (EC of ~21.1 mS/m) with a similar overall hydrochemical signature compared to the groundwater sample (WKQ_HBh2).

When comparing the results of the two water it is clear that the water collected from the quarry is clearly evaporation/precipitation dominated (concentrating effect, slightly elevated EC and enriched in Na relative to Ca) and the groundwater is rock dominated (equilibrium reactions with host rock minerals and enriched in Ca relative to Na). The results are displays in the Gibbs diagram below (**Figure 7**).

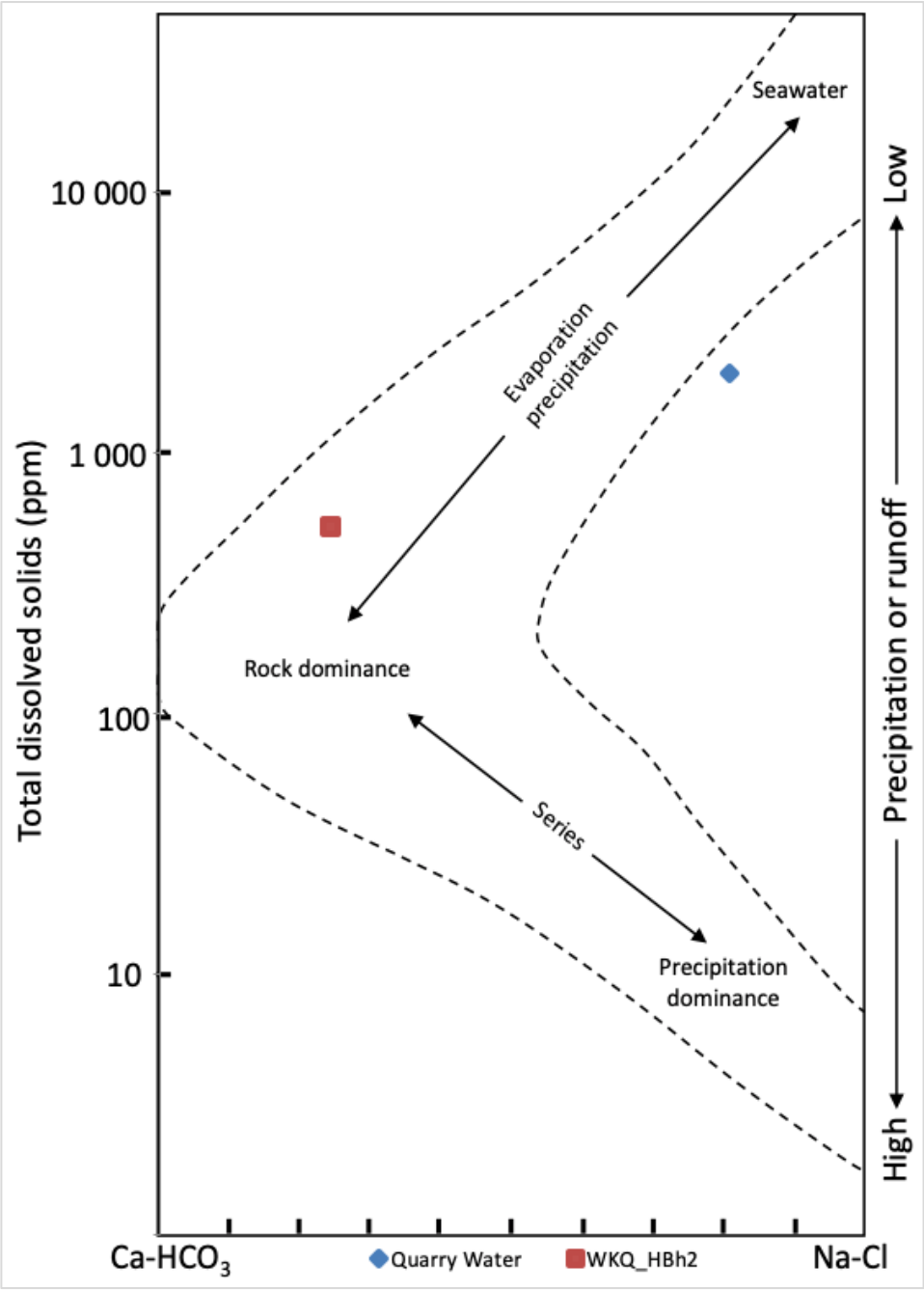


Figure 7: Gibb's diagram of the two water samples.

6. RISK ASSESSMENT

To evaluate potential risks at the site, the potential sources, pathways and receptors are considered.

6.1 Sources

The main possible contamination source relates to nitrates that are introduced into the quarry and the residing water from the blasting activities which are to take place. The quarry water/pit lake water is considered to be waste water and may be used as dust suppression.

Another source of contamination are hydrocarbons from leaking machinery and equipment. The oils and fuel from the various machinery may enter the subsurface should they be damaged or not suitably maintained and thus leak.

6.2 Pathways

The site overlies a fractured aquifer with a classified yield of 5 L/s. This fractured aquifer is made up of fractured Katberg Formation Sandstones and to a lessor extent the lower permeable mudstones of the Beaufort Group. The quarry itself is located on massive dolerite of low permeability. Therefore, the infiltration rate and transmissivity within the targeted dolerite is considered low.

The trucks that spray water on the grounds are a pathway for nitrate contamination to enter the groundwater, however very low infiltration is expected into the subsurface of the gravel roads. The quarry itself is also a pathway of contamination to possibly enter the groundwater system. The blasting activity within the quarry increases the fracturing of the rock in the walls and floor of the quarry. This could result in increased infiltration into the dolerite.

6.3 Receptors

In terms of groundwater users in the 1 km area, very few boreholes were identified. The main reason for this is the low yields in the dolerite itself and long distance to arable land. Even if there was groundwater use in the area, the risk of contamination from the quarry with pit lake water would still be low due to the impermeable nature of the bedrock.

6.4 Risk & Impact Assessment

Given the presence of sources, pathways and potential receptors, the risks and impacts are assessed in more detail. The risk associated to groundwater pertains to the operational mining phase only. The operational phase with potential sources relates to nitrates from blasting, leaking of hydrocarbons from machinery and dust suppression with rainwater infill (pit lake water).

It is important to note that the pit lake water (Quarry Water) is considered as waste water and is of poorer quality than the natural groundwater in terms of nitrate, sulphate and sodium. However, for some of the remainder of parameters tested for in this study, it was shown that the quarry water is of better-quality water than then surrounding groundwater in terms of magnesium, iron and copper.

Contamination of the fractured aquifer is unlikely to occur due to the low permeability of the massive dolerite. However, it is was seen that the water within the pit lakes does have elevated concentrations of nitrate, sulphate and sodium, and contamination of natural surface water bodies will occur if the quarry water is disposed in drainage channels.

Table 9 presents a summary of possible impacts associated with leaking hydrocarbons from machinery and vehicles during the operational phase. **Table 10** presents a summary of possible impacts associated with re-use of pit lake water as dust suppressant. The impacts listed are applicable to only the operational phase of the site.

Table 9: Impact table for assessing impact of leaking hydrocarbons from machinery and vehicles.

Construction Phase	
Potential impact and risk:	**Fuel loss and oil spill from construction vehicles and equipment contaminating groundwater**
Nature of impact:	Negative
Extent and duration of impact:	Extent is local and short term
Consequence of impact or risk:	Contamination to soil
Probability of occurrence:	Probable
Degree to which the impact may cause irreplaceable loss of resources:	Low
Degree to which the impact can be reversed:	Can be managed and mitigated
Cumulative impact prior to mitigation:	Very low
Significance rating of impact prior to mitigation (e.g., Low, Medium, Medium-High, High, or Very-High)	Low
Proposed mitigation:	Neat and tidy construction operation. Vehicles must be maintained regularly and kept in a good working order. Contaminated water and soil should be captured and disposed of off-site. No heavy equipment or vehicles to be left in close proximity to drainage channels. Standing vehicles at and proximal to the site must have drip trays.
Residual impacts:	No residual impact expected
Cumulative impact post mitigation:	None
Significance rating of impact after mitigation (e.g., Low, Medium, Medium-High, High, or Very-High)	Low

Table 10: Impact table for re-use of quarry water as dust suppression.

OPERATIONAL PHASE	
Potential impact and risk:	**Contamination of groundwater due to re-use of quarry water as dust suppression.**
Nature of impact:	Negative
Extent and duration of impact:	Extent is local and duration operational life.
Consequence of impact or risk:	Potential contamination to groundwater and soil
Probability of occurrence:	Low
Degree to which the impact may cause irreplaceable loss of resources:	Low
Degree to which the impact can be reversed:	Medium
Significance rating of impact prior to mitigation (e.g., Low, Medium, Medium-High, High, or Very-High)	Low
Degree to which the impact can be managed or mitigated:	High. Infiltration of access roads and operational which may need dust suppression is low.
Proposed mitigation:	Dust suppression: Water used for dust suppression will evaporate before it enters the groundwater system. No mitigation
Significance rating of impact after mitigation (e.g., Low, Medium, Medium-High, High, or Very-High)	Very Low

7. ASSUMPTIONS AND LIMITATIONS

During this study, certain assumptions limited the certainty of the data acquired and the outcome of this report.

- The groundwater quality was determined from one set of test results. Seasonal changes may occur in the chemistry of the water from the pit lakes, groundwater and stream which could not be accounted for.
- The coordinates of the NGA boreholes are sometimes found to be inaccurate. Hence, it was difficult to incorporate the NGA data accurately into the field hydrocensus.

8. CONCLUSION AND RECOMMENDATIONS

A geohydrological assessment was conducted on the Wolvekop Quarry to assess what the potential impact of proposed activities will have on the groundwater of the area.

The proposed activities are:

- Drilling and blasting the hard rock after the topsoil of the area has been stripped and stockpiled
- Load and haul the material out of the excavation to the crushing and screening plants
- Crush and screen the recovered material at the crusher plant in order to reduce it to various size aggregate,
- Stockpile the aggregate at a stockpile area until it is collected by clients.

The site overlies a fractured aquifer with a classified yield of 5 L/s (**Map 3**). This fractured aquifer is made up of fractured bedrock of the Katberg Formation. This comprises fractured sandstone and mudstone in close contact to dolerite intrusions (the periphery of dolerite). The groundwater quality based on regional data sets and onsite data is good (EC: <70 mS/m) resulting in a high degree of groundwater use in the low rainfall area (average is 320 mm/a).

Given the low to medium vulnerability of the aquifer, together with the above-mentioned factors, **the risk of potential contamination due to the proposed activities to the fractured aquifer is considered to be low**. It will however be important to ensure best management practices are implemented to avoid any unnecessary contamination from occurring.

There are however sources of potential contamination and these should be avoided regardless of the low/medium aquifer vulnerability rating. Recommendations for this are presented below:

Recommendation:
From a geohydrological prospective activities of the Wolvekop Quarry will have a minimal impact on the groundwater of the area. As the Quarry Water (rainfall held within the excavation) is of poorer quality than the surrounding groundwater with regards to elevated sodium, nitrates, and sulphates, unnecessary discharge into any proximal drainage channels should be avoided. The water can be used for dust suppression when and if necessary, as the water will evaporate before infiltration in to the hard, and low permeability bedrock below the quarry site area.

9. REFERENCES

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10. APPENDIX A: LABORATORY ANALYSIS

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TEST REPORT

Water

Distillery Road
Stellenbosch
Tel 021-8828866/7
info@vinlab.com
www.vinlab.com
2021-06-15

Geoss South Africa (Pty) Ltd
Attn: - Alison

P.O.Box 12412
Die Boord, Stellenbosch
7613
-
0218801079

@VinlabSA

Sample Details								
SampleID			W18821	W18822				
Water Type			Drinking Water	Drinking Water				
Water Source			Borehole					
Sample Temperature								
Description			Quarry Water	WKQ_HBh2				
PO Number			4332PhA	4332PhA				
Date Received			2021-06-10	2021-06-10				
Condition			Good	Good				
Water - Routine								
pH@25C* (Water)		VIN-05-MW01	>= 5 to <= 9.7	8.16	7.36			
Conductivity@25C* (Water)	mS/m	VIN-05-MW02	<= 170	298	76.8			
Turbidity (Water)	ntu		<= 5	1.20	2.10			
Total dissolved solids (Water)	mg/L		<= 1200	2020.44	520.70			
Free Chlorine (Water)	mg/L		<= 5	<0.02	<0.02			
Ammonia (NH4) as N* (Water)	mg/L	VIN-05-MW08	<= 1.5	<0.15	<0.15			
Nitrate as N* (Water)	mg/L	VIN-05-MW08	<= 11	57.84	5.08			
Nitrite as N* (Water)	mg/L	VIN-05-MW08	<= 0.9	0.06	<0.05			
Chloride (Cl-)* - Water	mg/L	VIN-05-MW08	<= 300	72.88	19.99			
Sulphates (SO4)* - Water	mg/L	VIN-05-MW08	<= 500	1220.08	63.01			
Fluoride (F)* - Water	mg/L	VIN-05-MW08	<= 1.5	0.51	0.43			
Alkalinity as CaCO3 (Water)	mg/L			62.50	312.40			
Colour (Water)	mg/L Pt-Co		<= 15	<15	<15			
Total Organic Carbon (Water)	mg/L		<=10	2.06	1.06			
Date Tested				2021-06-10	2021-06-10			
Water - Metals								
Calcium* (Ca) - Water	mg/L	VIN-05-MW43		124	71			
Magnesium* (Mg) - Water	mg/L	VIN-05-MW43		9	39			
Sodium* (Na) - Water	mg/L	VIN-05-MW43	<= 200	532	23			
Potassium* (K) - Water	mg/L	VIN-05-MW43		4	1			
Zinc* (Zn) - Water	mg/L	VIN-05-MW43	<= 5	<0.008	0.040			
Antimony (Sb) - Water	µg/L		<=13	16	<13.0			

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Test results relate only to the items tested as received. This Document shall not be reproduced without the written approval of Vinlab (Pty) Ltd.Opinions and interpretations expressed herein are outside
the scope of SANAS accreditation. Results for methods VIN-05-MW12, 13 and 14, are based on Cq values, a positive result (detected) indicates a Cq value <35 and a negative result (non-detected) indicates a Cq value of >35.

*Accredited methods. Vinlab is not liable to any client for any loss or damages suffered which could, directly or remotely, be linked to our services Alcohol results are obtained using the most appropriate or a combination of one of the following methods: Py= pycnometer; W=winescan; Al=alcolyzer. W = Winescan. Micro results: Enumeration of yeast: WL nutrient, 3 days unless otherwise specified, 30°C. Samples that have had prior microbiological spoilage or treatment for spoilage should always be sterile filtered at bottling. SO2 additions less than 10 days may depress the growth of microbes in culture although they are viable/active in the wine. Some microbes, especially lactobacilli, may not grow in culture even where viable/potentially active in the wine.

VIN 09-01 07-06-2021

Doc No
V27083

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2021-06-15

TEST REPORT

Water

@VinlabSA

Geoss South Africa (Pty) Ltd

Attn: - Alison

P.O.Box 12412
Die Boord, Stellenbosch
7613
-

0218801079

Arsenic (As) - Water	µg/L		<= 10	51	<10.0			
Boron (B)* Water	µg/L	VIN-05-MW43	<= 2400	888	103			
Cadmium (Cd)* Water	µg/L	VIN-05-MW43	<= 3	1	1			
Chromium* (Cr) - Water	µg/L	VIN-05-MW43	<= 50	<4	<4			
Copper* (Cu) - Water	µg/L	VIN-05-MW43	<= 2000	13	24			
Iron* (Fe) - Water	µg/L	VIN-05-MW43	<= 2000	12	244			
Lead* (Pb) - Water	µg/L	VIN-05-MW43	<= 10	8	<8			
Manganese* (Mn) - Water	µg/L	VIN-05-MW43	<= 400	<4	5			
Nickel* (Ni) - Water	µg/L	VIN-05-MW43	<= 70	<8	<8			
Selenium (Se) - Water	µg/L		<= 40	<10.0	<10.0			
Aluminium* (Al) - Water	µg/L	VIN-05-MW43	<= 300	28	11			
Cyanide (CN) - Water	µg/L		<= 200	<10.0	<10.0			
Mercury (Hg) - Water	µg/L		<= 6	<1.0	<1.0			
Barium (Ba)* Water	µg/L	VIN-05-MW43	<= 700	<8	25			
Uranium (U) - Water	µg/L		<= 30	<28	<28			
Date Tested				2021-06-14	2021-06-10			

Comments
W18821 Two Samples received, Ion balance = 3.9%
W18822 Two Samples received, Ion balance = 2.2%

Adelize Fourie
Laboratory Manager (Waterlab)
VIN-05-
M01,M02,M03,M04,M05,MC8,M10,M28,
M43, MW01, MW02, MW03, MW04,
MW05, MW06, MW07, MW08/9/10

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VIN 09-01 07-06-2021

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V27083

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APPENDIX B: PHREEQC OUTPUT DATA

Input file: \\Mac\Home\4332_Afrimat\

4332_Afrimat_Middelburg_01Jul2021_ce.pqi
Output file: \\Mac\Home\Music\4332_Afrimat\
4332_Afrimat_Middelburg_01Jul2021_ce.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\database\llnl.dat

---
Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

```
DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\database\llnl.dat
SOLUTION 1
   temp      25
   pH        7
   pe        4
   redox     pe
   units     mg/l
   density   1
   water     1 # kg
EQUILIBRIUM_PHASES 1
   CO2(g)    -3.387 10
   O2(g)     -0.679 10
SAVE solution 2
END
```

Beginning of initial solution calculations.

Initial solution 1.

----------Solution composition----------

Elements	Molality	Moles

Pure water

----------Description of solution----------

```
                                pH  =   7.000
                                pe  =   4.000
                     Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   9.823e-08
                      Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =  -3.654e-09
                       Temperature (°C)  =  25.00
                  Electrical balance (eq)  =   3.654e-09
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   1.86
                            Iterations  =   0
                              Total H  = 1.110507e+02
                              Total O  = 5.552533e+01
```

----------Distribution of species----------

Species	Molality	Log Activity	Log Molality	Log Activity	Gamma	mole V cm³/mol
H+	1.001e-07	1.000e-07	-7.000	-7.000	-0.000	0.00
OH-	9.640e-08	9.636e-08	-7.016	-7.016	-0.000	(0)
H2O	5.553e+01	1.000e+00	1.744	0.000	0.000	18.07
H(0)	1.587e-25					
H2	7.935e-26	7.935e-26	-25.100	-25.100	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-41.995	-41.995	0.000	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(298 K, 1 atm)
H2(g)	-22.00	-25.10	-3.10 H2
H2O(g)	-1.59	0.00	1.59 H2O
Ice	-0.14	0.00	0.14 H2O
O2(g)	-39.10	-42.00	-2.89 O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.

----------Phase assemblage----------

Phase	SI	log IAP	log K(T, P)	Moles in assemblage Initial	Final	Delta
CO2(g)	-3.39	-11.22	-7.83	1.000e+01	1.000e+01	-1.658e-05
O2(g)	-0.68	-3.57	-2.89	1.000e+01	1.000e+01	-2.683e-04

----------Solution composition----------

Elements	Molality	Moles
C	1.658e-05	1.658e-05

----------Description of solution----------

pH = 5.607 Charge balance
pe = 14.999 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength (mol/kgw) = 2.474e-06
Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = -3.654e-09
Total CO2 (mol/kg) = 1.658e-05
Temperature (°C) = 25.00
Electrical balance (eq) = 3.654e-09
Percent error, 100*(Cat- | An |)/(Cat+ | An |) = 0.07
Iterations = 11
Total H = 1.110507e+02
Total O = 5.552589e+01

----------Distribution of species----------

Log Log Log mole V

Species	Molality	Activity	Molality	Activity	Gamma	cm³/mol
H+	2.475e-06	2.471e-06	-5.606	-5.607	-0.001	0.00
OH-	3.907e-09	3.899e-09	-8.408	-8.409	-0.001	(0)
H2O	5.553e+01	1.000e+00	1.744	-0.000	0.000	18.07
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-266.135	-266.135	0.000	(0)
C(-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-260.013	-260.013	0.000	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-148.164	-148.164	0.000	(0)
C(2)	0.000e+00					
CO	0.000e+00	0.000e+00	-51.104	-51.104	0.000	(0)
C(4)	1.658e-05					
CO2	1.412e-05	1.412e-05	-4.850	-4.850	0.000	(0)
HCO3-	2.468e-06	2.463e-06	-5.608	-5.609	-0.001	(0)
CO3-2	4.456e-11	4.423e-11	-10.351	-10.354	-0.003	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-44.312	-44.312	0.000	(0)
O(0)	5.366e-04					
O2	2.683e-04	2.683e-04	-3.571	-3.571	0.000	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
C	-71.79	-7.64	64.15	C
C(g)	-189.41	-7.64	181.77	C
CH4(g)	-145.32	-148.16	-2.84	CH4
CO(g)	-48.11	-51.10	-3.00	CO
CO2(g)	-3.39	-11.22	-7.83	CO2
H2(g)	-41.21	-44.31	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Ice	-0.14	-0.00	0.14	H2O
O2(g)	-0.68	-3.57	-2.89	O2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

```
USE solution 2
EQUILIBRIUM_PHASES 2
   Albite    0 10
   Anorthite 0 10
   Ca-Al_Pyroxene 0 10
   Diopside  0 10
   Hedenbergite 0 10
   Pargasite 0 10
   Fayalite  0 10
   Forsterite 0 10
   Magnetite 0 10
   Quartz    0 10
END
```

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 2. Solution after simulation 1.

Using pure phase assemblage 2.

----------Phase assemblage----------

Phase	SI	log IAP	log K(T, P)	Moles in assemblage Initial	Final	Delta
Albite	0.00	2.66	2.66	1.000e+01	6.667e+00	-3.333e+00
Anorthite	0.00	26.48	26.48	1.000e+01	1.667e+01	6.666e+00
Ca-Al_Pyroxene	-5.40	30.50	35.90	1.000e+01	0	-1.000e+01
Diopside	0.00	20.89	20.89	1.000e+01	1.667e+01	6.668e+00
Fayalite	0.00	19.06	19.06	1.000e+01	1.500e+01	4.999e+00
Forsterite	-0.07	27.74	27.81	1.000e+01	0	-1.000e+01
Hedenbergite	-2.98	16.55	19.53	1.000e+01	0	-1.000e+01
Magnetite	-0.00	10.42	10.42	1.000e+01	1.000e+01	6.142e-04
Pargasite	0.00	101.70	101.70	1.000e+01	1.333e+01	3.333e+00
Quartz	0.00	-4.03	-4.03	1.000e+01	8.333e+00	-1.667e+00

----------Solution composition----------

Elements	Molality	Moles
Al	2.211e-03	2.078e-03
C	1.764e-05	1.658e-05
Ca	1.705e-06	1.603e-06
Fe	9.356e-08	8.795e-08
Mg	1.132e-03	1.064e-03
Na	3.679e-06	3.458e-06
Si	1.272e-04	1.196e-04

----------Description of solution----------

pH = 9.466 Charge balance
pe = -8.555 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength (mol/kgw) = 3.406e-03
Mass of water (kg) = 9.400e-01
Total alkalinity (eq/kg) = 8.903e-03
Total CO2 (mol/kg) = 1.736e-16
Temperature (°C) = 25.00
Electrical balance (eq) = 3.647e-09
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.00
Iterations = 30
Total H = 1.043854e+02
Total O = 5.219707e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	3.006e-05	2.820e-05	-4.522	-4.550	-0.028	(0)
H+	3.622e-10	3.417e-10	-9.441	-9.466	-0.025	0.00
H2O	5.553e+01	9.999e-01	1.744	-0.000	0.000	18.07
Al	2.211e-03					
AlO2-	2.208e-03	2.073e-03	-2.656	-2.683	-0.028	(0)
HAlO2	2.067e-06	2.067e-06	-5.685	-5.685	0.000	(0)
NaAlO2	1.363e-09	1.363e-09	-8.866	-8.866	0.000	(0)
Al(OH)2+	5.171e-10	4.853e-10	-9.286	-9.314	-0.028	(0)
AlOH+2	9.195e-14	7.142e-14	-13.036	-13.146	-0.110	(0)
Al+3	3.690e-18	2.178e-18	-17.433	-17.662	-0.229	(0)
Al2(OH)2+4	2.242e-24	8.294e-25	-23.649	-24.081	-0.432	(0)
Al13O4(OH)24+7	7.953e-25	3.884e-26	-24.099	-25.411	-1.311	(0)
Al3(OH)4+5	4.661e-29	9.989e-30	-28.332	-29.000	-0.669	(0)
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-58.092	-58.092	0.000	(0)
C(-3)	5.250e-13					

```
   C2H6          2.625e-13   2.625e-13   -12.581   -12.581     0.000     (0)
C(-4)         1.764e-05
   CH4           1.764e-05   1.764e-05    -4.753    -4.753     0.000     (0)
C(2)          1.376e-26
   CO            1.376e-26   1.376e-26   -25.861   -25.861     0.000     (0)
C(4)          1.736e-16
   HCO3-         1.352e-16   1.269e-16   -15.869   -15.897    -0.028     (0)
   CO3-2         2.121e-17   1.647e-17   -16.673   -16.783    -0.110     (0)
   MgCO3         1.555e-17   1.555e-17   -16.808   -16.808     0.000     (0)
   MgHCO3+       1.401e-18   1.315e-18   -17.853   -17.881    -0.028     (0)
   CO2           1.005e-19   1.006e-19   -18.998   -18.998     0.000     (0)
   CaCO3         5.087e-20   5.087e-20   -19.294   -19.294     0.000     (0)
   FeCO3         3.822e-20   3.822e-20   -19.418   -19.418     0.000     (0)
   FeHCO3+       2.900e-21   2.721e-21   -20.538   -20.565    -0.028     (0)
   CaHCO3+       2.135e-21   2.003e-21   -20.671   -20.698    -0.028     (0)
   NaHCO3        6.255e-22   6.255e-22   -21.204   -21.204     0.000     (0)
   NaCO3-        2.117e-22   1.987e-22   -21.674   -21.702    -0.028     (0)
   FeCO3+        1.106e-36   1.038e-36   -35.956   -35.984    -0.028     (0)
Ca            1.705e-06
   Ca+2          1.704e-06   1.332e-06    -5.768    -5.875    -0.107     (0)
   CaOH+         5.869e-10   5.508e-10    -9.231    -9.259    -0.028     (0)
   CaCO3         5.087e-20   5.087e-20   -19.294   -19.294     0.000     (0)
   CaHCO3+       2.135e-21   2.003e-21   -20.671   -20.698    -0.028     (0)
Fe(2)         9.356e-08
   Fe+2          5.227e-08   4.087e-08    -7.282    -7.389    -0.107     (0)
   FeOH+         4.030e-08   3.782e-08    -7.395    -7.422    -0.028     (0)
   Fe(OH)2       8.792e-10   8.792e-10    -9.056    -9.056     0.000     (0)
   Fe(OH)3-      1.092e-10   1.024e-10    -9.962    -9.990    -0.028     (0)
   Fe(OH)4-2     3.869e-16   2.998e-16   -15.412   -15.523    -0.111     (0)
   FeCO3         3.822e-20   3.822e-20   -19.418   -19.418     0.000     (0)
   FeHCO3+       2.900e-21   2.721e-21   -20.538   -20.565    -0.028     (0)
Fe(3)         4.879e-13
   Fe(OH)3       2.735e-13   2.735e-13   -12.563   -12.563     0.000     (0)
   Fe(OH)4-      2.142e-13   2.010e-13   -12.669   -12.697    -0.028     (0)
   Fe(OH)2+      2.129e-16   1.998e-16   -15.672   -15.699    -0.028     (0)
   FeOH+2        2.654e-22   2.062e-22   -21.576   -21.686    -0.110     (0)
   Fe+3          1.848e-29   1.091e-29   -28.733   -28.962    -0.229     (0)
   FeCO3+        1.106e-36   1.038e-36   -35.956   -35.984    -0.028     (0)
   Fe2(OH)2+4    0.000e+00   0.000e+00   -41.510   -41.942    -0.432     (0)
   Fe3(OH)4+5    0.000e+00   0.000e+00   -54.652   -55.321    -0.669     (0)
H(0)          2.387e-05
   H2            1.194e-05   1.195e-05    -4.923    -4.923     0.000     (0)
Mg            1.132e-03
   Mg+2          1.132e-03   8.925e-04    -2.946    -3.049    -0.103     (0)
   Mg4(OH)4+4    2.237e-14   8.278e-15   -13.650   -14.082    -0.432     (0)
   MgCO3         1.555e-17   1.555e-17   -16.808   -16.808     0.000     (0)
   MgHCO3+       1.401e-18   1.315e-18   -17.853   -17.881    -0.028     (0)
Na            3.679e-06
   Na+           3.673e-06   3.447e-06    -5.435    -5.463    -0.028     (0)
   NaHSiO3       5.091e-09   5.091e-09    -8.293    -8.293     0.000     (0)
   NaAlO2        1.363e-09   1.363e-09    -8.866    -8.866     0.000     (0)
   NaOH          1.677e-11   1.677e-11   -10.776   -10.776     0.000     (0)
   NaHCO3        6.255e-22   6.255e-22   -21.204   -21.204     0.000     (0)
   NaCO3-        2.117e-22   1.987e-22   -21.674   -21.702    -0.028     (0)
O(0)          0.000e+00
   O2            0.000e+00   0.000e+00   -82.351   -82.351     0.000     (0)
Si            1.272e-04
   SiO2          9.379e-05   9.379e-05    -4.028    -4.028     0.000     (0)
   HSiO3-        3.341e-05   3.135e-05    -4.476    -4.504    -0.028     (0)
   H2SiO4-2      1.137e-08   8.808e-09    -7.944    -8.055    -0.111     (0)
   NaHSiO3       5.091e-09   5.091e-09    -8.293    -8.293     0.000     (0)
   H6(H2SiO4)4-2 1.958e-11   1.518e-11   -10.708   -10.819    -0.111     (0)
   H4(H2SiO4)4-4 1.808e-14   6.515e-15   -13.743   -14.186    -0.443     (0)

-------------------------------Saturation indices-------------------------------

  Phase               SI** log IAP   log K(298 K,   1 atm)
```

Afwillite -28.85 31.12 59.96 Ca3Si2O4(OH)6
Akermanite -11.29 33.94 45.23 Ca2MgSi2O7
Al -77.41 72.50 149.91 Al
Al(g) -128.12 72.50 200.62 Al
Albite 0.00 2.66 2.66 NaAlSi3O8
Albite_high -1.32 2.66 3.98 NaAlSi3O8
Albite_low -0.00 2.66 2.66 NaAlSi3O8
Amesite-14A 23.15 98.43 75.27 Mg4Al4Si2O10(OH)8
Analcime -0.12 5.93 6.06 Na.96Al.96Si2.04O6:H2O
Analcime-dehy -6.49 5.93 12.42 Na.96Al.96Si2.04O6
Andalusite 1.57 17.45 15.88 Al2SiO5
Andradite -7.22 25.96 33.19 Ca3Fe2(SiO4)3
Anorthite 0.00 26.48 26.48 CaAl2(SiO4)2
Anthophyllite 12.48 78.96 66.48 Mg7Si8O22(OH)2
Antigorite 149.82 625.45 475.63 Mg48Si34O85(OH)62
Aragonite -14.28 -12.31 1.97 CaCO3
Artinite -13.22 6.40 19.63 Mg2CO3(OH)2:3H2O
Beidellite-Ca 6.95 12.39 5.44 Ca.165Al2.33Si3.67O10(OH)2
Beidellite-H 5.75 10.24 4.49 H.33Al2.33Si3.67O10(OH)2
Beidellite-Mg 7.45 12.86 5.41 Mg.165Al2.33Si3.67O10(OH)2
Beidellite-Na 6.06 11.56 5.50 Na.33Al2.33Si3.67O10(OH)2
Boehmite 3.19 10.74 7.55 AlO2H
Brucite -0.40 15.88 16.28 Mg(OH)2
C -7.16 56.99 64.15 C
C(g) -124.78 56.99 181.77 C
Ca -85.60 54.23 139.83 Ca
Ca(g) -110.84 54.23 165.07 Ca
Ca-Al_Pyroxene -5.40 30.50 35.90 CaAl2SiO6
Ca2Al2O5:8H2O -11.98 47.59 59.57 Ca2Al2O5:8H2O
Ca3Al2O6 -52.38 60.65 113.03 Ca3Al2O6
Ca4Al2Fe2O10 -67.90 72.58 140.48 Ca4Al2Fe2O10
Ca4Al2O7:13H2O -33.55 73.70 107.25 Ca4Al2O7:13H2O
Ca4Al2O7:19H2O -29.98 73.70 103.68 Ca4Al2O7:19H2O
CaAl2O4 -12.38 34.53 46.91 CaAl2O4
CaAl2O4:10H2O -3.46 34.53 37.99 CaAl2O4:10H2O
CaAl4O7 -12.58 56.01 68.59 CaAl4O7
Calcite -14.13 -12.31 1.82 CaCO3
CH4(g) -1.91 -4.75 -2.84 CH4
Chalcedony -0.27 -4.03 -3.76 SiO2
Chamosite-7A 7.78 40.53 32.76 Fe2Al2SiO5(OH)4
Chrysotile 8.56 39.59 31.03 Mg3Si2O5(OH)4
Clinochlore-14A 21.76 88.81 67.05 Mg5Al2Si3O10(OH)8
Clinochlore-7A 18.38 88.81 70.42 Mg5Al2Si3O10(OH)8
Clinoptilolite-Ca 8.65 1.13 -7.52 Ca1.7335Al3.45Fe.017Si14.533O36:10.922H2O
Clinoptilolite-dehy-Ca -27.01 1.13 28.14 Ca1.7335Al3.45Fe.017Si14.533O36
Clinoptilolite-dehy-Na -35.63 -7.62 28.01 Na3.467Al3.45Fe.017Si14.533O36
Clinoptilolite-hy-Ca 8.65 1.13 -7.52 Ca1.7335Al3.45Fe.017Si14.533O36:11.645H2O
Clinoptilolite-hy-Na 0.02 -7.62 -7.65 Na3.467Al3.45Fe.017Si14.533O36:10.877H2O
Clinoptilolite-Na 0.02 -7.62 -7.64 Na3.467Al3.45Fe.017Si14.533O36:10.922H2O
Clinozoisite 3.14 46.24 43.10 Ca2Al3Si3O12(OH)
CO(g) -22.86 -25.86 -3.00 CO
CO2(g) -17.53 -25.36 -7.83 CO2
Coesite -0.81 -4.03 -3.22 SiO2
Cordierite_anhyd 2.51 54.58 52.07 Mg2Al4Si5O18
Cordierite_hydr 4.99 54.58 49.59 Mg2Al4Si5O18:H2O
Corundum 3.18 21.47 18.29 Al2O3
Cristobalite(alpha) -0.55 -4.03 -3.48 SiO2
Cristobalite(beta) -0.99 -4.03 -3.03 SiO2
Cronstedtite-7A 1.76 17.93 16.18 Fe2Fe2SiO5(OH)4
Daphnite-14A 15.01 67.11 52.10 Fe5AlAlSi3O10(OH)8
Daphnite-7A 11.64 67.11 55.48 Fe5AlAlSi3O10(OH)8
Dawsonite -14.96 -10.62 4.34 NaAlCO3(OH)2
Diaspore 3.59 10.74 7.15 AlHO2
Dicalcium_silicate -15.04 22.09 37.13 Ca2SiO4
Diopside 0.00 20.89 20.89 CaMgSi2O6
Dolomite -24.26 -21.79 2.47 CaMg(CO3)2

Dolomite-dis	-25.80	-21.79	4.01	CaMg(CO3)2
Dolomite-ord	-24.25	-21.79	2.46	CaMg(CO3)2
Enstatite	0.57	11.86	11.29	MgSiO3
Epidote	2.17	34.94	32.77	Ca2FeAl2Si3O12OH
Epidote-ord	2.18	34.94	32.76	FeCa2Al2(OH)(SiO4)3
Fayalite	0.00	19.06	19.06	Fe2SiO4
Fe	-6.30	52.72	59.02	Fe
Fe(OH)2	-2.35	11.54	13.89	Fe(OH)2
Fe(OH)3	-6.20	-0.56	5.64	Fe(OH)3
FeO	-1.98	11.54	13.52	FeO
Ferrite-Ca	-9.56	11.93	21.50	CaFe2O4
Ferrite-Dicalcium	-31.81	24.99	56.80	Ca2Fe2O5
Ferrite-Mg	-6.26	14.76	21.02	MgFe2O4
Ferrosilite	0.11	7.52	7.41	FeSiO3
Forsterite	-0.07	27.74	27.81	Mg2SiO4
Foshagite	-25.65	40.15	65.80	Ca4Si3O9(OH)2:0.5H2O
Gaylussite	-40.83	-29.66	11.16	CaNa2(CO3)2:5H2O
Gehlenite	-12.66	43.56	56.22	Ca2Al2SiO7
Gibbsite	3.00	10.74	7.74	Al(OH)3
Gismondine	11.24	52.95	41.72	Ca2Al4Si4O16:9H2O
Goethite	-1.09	-0.56	0.53	FeOOH
Greenalite	4.00	26.58	22.58	Fe3Si2O5(OH)4
Grossular	-3.21	48.56	51.78	Ca3Al2(SiO4)3
Gyrolite	-8.77	14.03	22.80	Ca2Si3O7(OH)2:1.5H2O
H2(g)	-1.82	-4.92	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Hatrurite	-38.21	35.14	73.35	Ca3SiO5
Hedenbergite	-2.98	16.55	19.53	CaFe(SiO3)2
Hematite	-1.20	-1.13	0.08	Fe2O3
Hercynite	4.22	33.02	28.80	FeAl2O4
Hillebrandite	-14.68	22.09	36.77	Ca2SiO3(OH)2:0.17H2O
Huntite	-50.96	-40.74	10.22	CaMg3(CO3)4
Hydromagnesite	-52.77	-22.04	30.74	Mg5(CO3)4(OH)2:4H2O
Ice	-0.14	-0.00	0.14	H2O
Jadeite	-1.62	6.69	8.31	NaAl(SiO3)2
Kaolinite	6.70	13.42	6.72	Al2Si2O5(OH)4
Katoite	-18.30	60.65	78.94	Ca3Al2H12O12
Kyanite	1.84	17.45	15.61	Al2SiO5
Lansfordite	-14.32	-9.48	4.84	MgCO3:5H2O
Larnite	-16.33	22.09	38.42	Ca2SiO4
Laumontite	4.91	18.42	13.51	CaAl2Si4O12:4H2O
Lawsonite	4.37	26.48	22.11	CaAl2Si2O7(OH)2:H2O
Lime	-19.51	13.06	32.57	CaO
Magnesite	-11.75	-9.48	2.27	MgCO3
Magnetite	-0.00	10.42	10.42	Fe3O4
Margarite	7.03	47.95	40.93	CaAl4Si2O10(OH)2
Mayenite	-187.14	307.01	494.15	Ca12Al14O33
Merwinite	-21.41	47.00	68.41	MgCa3(SiO4)2
Mesolite	7.04	20.53	13.49	Na.676Ca.657Al1.99Si3.01O10:2.647H2O
Mg	-65.46	57.06	122.52	Mg
Mg(g)	-85.19	57.06	142.25	Mg
Minnesotaite	4.69	18.52	13.83	Fe3Si4O10(OH)2
Monohydrocalcite	-14.98	-12.31	2.68	CaCO3:H2O
Monticellite	-4.62	24.91	29.53	CaMgSiO4
Montmor-Ca	6.87	9.22	2.34	Ca.165Mg.33Al1.67Si4O10(OH)2
Montmor-Mg	7.45	9.68	2.23	Mg.495Al1.67Si4O10(OH)2
Montmor-Na	6.05	8.38	2.33	Na.33Mg.33Al1.67Si4O10(OH)2
Mordenite	0.30	-5.06	-5.36	Ca.2895Na.361Al.94Si5.06O12:3.468H2O
Mordenite-dehy	-14.83	-5.06	9.77	Ca.2895Na.361Al.94Si5.06O12
Na	-42.78	24.59	67.37	Na
Na(g)	-56.27	24.59	80.86	Na
Na2CO3	-28.52	-17.36	11.16	Na2CO3
Na2CO3:7H2O	-27.29	-17.36	9.94	Na2CO3:7H2O
Na2O	-59.41	8.01	67.42	Na2O
Na2SiO3	-18.22	3.98	22.20	Na2SiO3
Na4SiO4	-58.61	11.99	70.60	Na4SiO4
Na6Si2O7	-85.56	15.97	101.53	Na6Si2O7

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NaFeO2          -16.44      3.44   19.88  NaFeO2
Nahcolite       -21.22    -21.36   -0.14  NaHCO3
Natrolite        -0.99     17.40   18.39  Na2Al2Si3O10:2H2O
Natron          -26.94    -17.36    9.59  Na2CO3:10H2O
Natrosilite     -18.11     -0.05   18.07  Na2Si2O5
Nepheline        -3.04     10.71   13.75  NaAlSiO4
Nesquehonite    -14.77     -9.48    5.29  MgCO3:3H2O
Nontronite-Ca     1.52    -10.21  -11.73  Ca.165Fe2Al.33Si3.67H2O12
Nontronite-H      0.33    -12.37  -12.69  H.33Fe2Al.33Si3.67H2O12
Nontronite-Mg     2.03     -9.74  -11.77  Mg.165Fe2Al.33Si3.67H2O12
Nontronite-Na     0.63    -11.04  -11.68  Na.33Fe2Al.33Si3.67H2O12
O2(g)           -79.46    -82.35   -2.89  O2
Okenite          -5.31      5.00   10.31  CaSi2O4(OH)2:H2O
Paragonite        6.75     24.13   17.38  NaAl3Si3O10(OH)2
Pargasite         0.00    101.70  101.70  NaCa2Al3Mg4Si6O22(OH)2
Periclase        -5.44     15.88   21.33  MgO
Pirssonite      -40.98    -29.66   11.32  Na2Ca(CO3)2:2H2O
Portlandite      -9.49     13.06   22.55  Ca(OH)2
Prehnite          2.71     35.51   32.79  Ca2Al2Si3O10(OH)2
Pseudowollastonite -4.93    9.03   13.96  CaSiO3
Pyrophyllite      5.07      5.36    0.29  Al2Si4O10(OH)2
Quartz            0.00     -4.03   -4.03  SiO2
Rankinite       -20.71     31.12   51.82  Ca3Si2O7
Ripidolite-14A   19.35     80.13   60.78  Mg3Fe2Al2Si3O10(OH)8
Ripidolite-7A    15.97     80.13   64.16  Mg3Fe2Al2Si3O10(OH)8
Saponite-Ca      12.42     38.57   26.14  Ca.165Mg3Al.33Si3.67O10(OH)2
Saponite-H       11.23     36.41   25.18  H.33Mg3Al.33Si3.67O10(OH)2
Saponite-Mg      12.93     39.03   26.10  Mg3.165Al.33Si3.67O10(OH)2
Saponite-Na      11.54     37.73   26.20  Na.33Mg3Al.33Si3.67O10(OH)2
Scolecite         6.70     22.45   15.75  CaAl2Si3O10:3H2O
Sepiolite         9.15     39.37   30.22  Mg4Si6O15(OH)2:6H2O
Si             -70.54     78.32  148.86  Si
Si(g)          -141.62     78.32  219.94  Si
Siderite       -13.60    -13.82   -0.22  FeCO3
Sillimanite      1.20     17.45   16.24  Al2SiO5
SiO2(am)        -1.29     -4.03   -2.74  SiO2
Spinel          -0.25     37.36   37.61  Al2MgO4
Talc            10.55     31.54   20.99  Mg3Si4O10(OH)2
Thermonatrite   -28.29    -17.36   10.94  Na2CO3:H2O
Tobermorite-11A -24.27     41.12   65.39  Ca5Si6H11O22.5
Tobermorite-14A -22.49     41.12   63.61  Ca5Si6H21O27.5
Tobermorite-9A  -27.74     41.12   68.86  Ca5Si6H6O20
Tremolite        12.38     73.31   60.93  Ca2Mg5Si8O22(OH)2
Tridymite        -0.19     -4.03   -3.84  SiO2
Wairakite         0.50     18.42   17.92  CaAl2Si4O10(OH)4
Wollastonite     -4.69      9.03   13.72  CaSiO3
Wustite          -2.75      9.65   12.40  Fe.947O
Xonotlite       -37.56     54.18   91.74  Ca6Si6O17(OH)2
Zoisite          3.11     46.24   43.14  Ca2Al3(SiO4)3OH

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 3.
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            SOLUTION 2 Quarry Water
              temp      25
              pH        8.16
              pe        4
              redox     pe
              units     mg/l
```

```
    density   1
    Al        28 ug/l
    Alkalinity 62.5
    As        51 ug/l
    B         888 ug/l
    Ca        124
    Cd        1 ug/l
    Cl        72.88
    Cu        13 ug/l
    F         0.51
    Fe        12 ug/l
    K         4
    Mg        9
    N(3)      0.06 as N
    N(5)      57.84 as N
    Na        532
    S(6)      1220.08 as SO4-2
    water     1 # kg
END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 2.         Quarry Water

-----------------------------Solution composition------------------------------

        Elements          Molality       Moles

        Al              1.040e-06   1.040e-06
        Alkalinity      1.252e-03   1.252e-03
        As              6.821e-07   6.821e-07
        B               8.231e-05   8.231e-05
        Ca              3.100e-03   3.100e-03
        Cd              8.915e-09   8.915e-09
        Cl              2.060e-03   2.060e-03
        Cu              2.050e-07   2.050e-07
        F               2.690e-05   2.690e-05
        Fe              2.153e-07   2.153e-07
        K               1.025e-04   1.025e-04
        Mg              3.711e-04   3.711e-04
        N(3)            4.293e-06   4.293e-06
        N(5)            4.138e-03   4.138e-03
        Na              2.319e-02   2.319e-02
        S(6)            1.273e-02   1.273e-02

----------------------------Description of solution----------------------------

                            pH  =   8.160
                            pe  =   4.000
                  Activity of water  =   0.999
             Ionic strength (mol/kgw)  =   4.213e-02
                Mass of water (kg)  =   1.000e+00
              Total carbon (mol/kg)  =   1.223e-03
                Total CO2 (mol/kg)  =   1.223e-03
                   Temperature (°C)  =  25.00
             Electrical balance (eq)  =  -2.704e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -4.71
                         Iterations  =  25
                            Total H  = 1.110521e+02
                            Total O  = 5.559257e+01

---------------------------------Redox couples---------------------------------

        Redox couple            pe  Eh (volts)

        N(3)/N(5)           7.2133      0.4267
```

----------Distribution of species----------

Species	Molality	Log Activity	Log Molality	Log Activity	Gamma	mole V cm³/mol
OH-	1.685e-06	1.392e-06	-5.773	-5.856	-0.083	(0)
H+	8.009e-09	6.918e-09	-8.096	-8.160	-0.064	0.00
H2O	5.553e+01	9.992e-01	1.744	-0.000	0.000	18.07
Al	1.040e-06					
AlO2-	1.020e-06	8.464e-07	-5.992	-6.072	-0.081	(0)
HAlO2	1.709e-08	1.709e-08	-7.767	-7.767	0.000	(0)
NaAlO2	3.001e-09	3.001e-09	-8.523	-8.523	0.000	(0)
Al(OH)2+	9.790e-11	8.126e-11	-10.009	-10.090	-0.081	(0)
AlOH+2	5.066e-13	2.423e-13	-12.295	-12.616	-0.320	(0)
AlF2+	3.299e-13	2.738e-13	-12.482	-12.562	-0.081	(0)
AlF3	7.389e-14	7.389e-14	-13.131	-13.131	0.000	(0)
AlF+2	6.711e-14	3.209e-14	-13.173	-13.494	-0.320	(0)
AlSO4+	9.498e-16	7.883e-16	-15.022	-15.103	-0.081	(0)
Al+3	5.772e-16	1.497e-16	-15.239	-15.825	-0.586	(0)
AlF4-	4.793e-16	3.978e-16	-15.319	-15.400	-0.081	(0)
Al(SO4)2-	3.793e-16	3.148e-16	-15.421	-15.502	-0.081	(0)
Al2(OH)2+4	1.596e-22	9.545e-24	-21.797	-23.020	-1.223	(0)
Al3(OH)4+5	1.414e-27	1.925e-29	-26.849	-28.716	-1.866	(0)
Al13O4(OH)24+7	2.086e-40	0.000e+00	-39.681	-43.340	-3.659	(0)
As(-3)	0.000e+00					
AsH3	0.000e+00	0.000e+00	-130.722	-130.722	0.000	(0)
As(3)	0.000e+00					
HAsO2	0.000e+00	0.000e+00	-52.815	-52.815	0.000	(0)
As(OH)3	0.000e+00	0.000e+00	-52.874	-52.874	0.000	(0)
H2AsO3-	0.000e+00	0.000e+00	-53.846	-53.927	-0.081	(0)
AsO2-	0.000e+00	0.000e+00	-53.865	-53.946	-0.081	(0)
AsO2OH-2	0.000e+00	0.000e+00	-56.448	-56.777	-0.329	(0)
As(5)	6.821e-07					
AsO3F-2	6.802e-07	3.189e-07	-6.167	-6.496	-0.329	(0)
HAsO3F-	1.974e-09	1.638e-09	-8.705	-8.786	-0.081	(0)
HAsO4-2	0.000e+00	0.000e+00	-40.364	-40.693	-0.329	(0)
H2AsO4-	0.000e+00	0.000e+00	-41.992	-42.073	-0.081	(0)
AsO4-3	0.000e+00	0.000e+00	-43.381	-44.124	-0.742	(0)
H3AsO4	0.000e+00	0.000e+00	-47.987	-47.987	0.000	(0)
B(-5)	0.000e+00					
BH4-	0.000e+00	0.000e+00	-158.260	-158.341	-0.081	(0)
B(3)	8.231e-05					
B(OH)3	7.452e-05	7.452e-05	-4.128	-4.128	0.000	(0)
BO2-	6.964e-06	5.780e-06	-5.157	-5.238	-0.081	(0)
CaB(OH)4+	5.466e-07	4.536e-07	-6.262	-6.343	-0.081	(0)
NaB(OH)4	2.124e-07	2.124e-07	-6.673	-6.673	0.000	(0)
MgB(OH)4+	6.639e-08	5.510e-08	-7.178	-7.259	-0.081	(0)
BF2(OH)2-	1.183e-15	9.822e-16	-14.927	-15.008	-0.081	(0)
B2O(OH)5-	1.997e-19	1.657e-19	-18.700	-18.781	-0.081	(0)
BF3OH-	7.491e-22	6.217e-22	-21.125	-21.206	-0.081	(0)
BF4-	7.368e-30	6.115e-30	-29.133	-29.214	-0.081	(0)
C(4)	1.223e-03					
HCO3-	1.137e-03	9.436e-04	-2.944	-3.025	-0.081	(0)
NaHCO3	2.509e-05	2.509e-05	-4.601	-4.601	0.000	(0)
CaCO3	1.563e-05	1.563e-05	-4.806	-4.806	0.000	(0)
CaHCO3+	1.501e-05	1.246e-05	-4.824	-4.905	-0.081	(0)
CO2	1.500e-05	1.515e-05	-4.824	-4.819	0.004	(0)
CO3-2	1.265e-05	6.051e-06	-4.898	-5.218	-0.320	(0)
MgHCO3+	1.502e-06	1.247e-06	-5.823	-5.904	-0.081	(0)
MgCO3	7.281e-07	7.281e-07	-6.138	-6.138	0.000	(0)
NaCO3-	4.742e-07	3.936e-07	-6.324	-6.405	-0.081	(0)
CuCO3	1.660e-07	1.660e-07	-6.780	-6.780	0.000	(0)
Cu(CO3)2-2	3.816e-09	1.789e-09	-8.418	-8.747	-0.329	(0)
CdHCO3+	1.013e-10	8.409e-11	-9.994	-10.075	-0.081	(0)
CuCO3(OH)2-2	6.278e-11	2.944e-11	-10.202	-10.531	-0.329	(0)
FeHCO3+	4.184e-11	3.473e-11	-10.378	-10.459	-0.081	(0)

FeCO3	2.409e-11	2.409e-11	-10.618	-10.618	0.000	(0)
CdCO3	1.803e-11	1.803e-11	-10.744	-10.744	0.000	(0)
Cd(CO3)2-2	6.178e-13	2.897e-13	-12.209	-12.538	-0.329	(0)
FeCO3+	2.831e-15	2.350e-15	-14.548	-14.629	-0.081	(0)
Ca	3.100e-03					
Ca+2	2.209e-03	1.114e-03	-2.656	-2.953	-0.297	(0)
CaSO4	8.373e-04	8.373e-04	-3.077	-3.077	0.000	(0)
CaNO3+	2.274e-05	1.887e-05	-4.643	-4.724	-0.081	(0)
CaCO3	1.563e-05	1.563e-05	-4.806	-4.806	0.000	(0)
CaHCO3+	1.501e-05	1.246e-05	-4.824	-4.905	-0.081	(0)
CaB(OH)4+	5.466e-07	4.536e-07	-6.262	-6.343	-0.081	(0)
CaCl+	4.799e-07	3.983e-07	-6.319	-6.400	-0.081	(0)
CaF+	1.463e-07	1.214e-07	-6.835	-6.916	-0.081	(0)
CaOH+	2.739e-08	2.273e-08	-7.562	-7.643	-0.081	(0)
CaCl2	7.901e-10	7.901e-10	-9.102	-9.102	0.000	(0)
Cd	8.915e-09					
Cd+2	5.783e-09	2.818e-09	-8.238	-8.550	-0.312	(0)
CdCl+	2.909e-09	2.415e-09	-8.536	-8.617	-0.081	(0)
CdHCO3+	1.013e-10	8.409e-11	-9.994	-10.075	-0.081	(0)
CdOH+	4.125e-11	3.424e-11	-10.385	-10.465	-0.081	(0)
Cd(OH)Cl	2.534e-11	2.534e-11	-10.596	-10.596	0.000	(0)
CdCO3	1.803e-11	1.803e-11	-10.744	-10.744	0.000	(0)
CdCl2	1.766e-11	1.766e-11	-10.753	-10.753	0.000	(0)
CdSO4	1.471e-11	1.471e-11	-10.832	-10.832	0.000	(0)
CdNO2+	2.806e-12	2.329e-12	-11.552	-11.633	-0.081	(0)
Cd(CO3)2-2	6.178e-13	2.897e-13	-12.209	-12.538	-0.329	(0)
Cd(OH)2	2.686e-13	2.686e-13	-12.571	-12.571	0.000	(0)
CdCl3-	9.203e-15	7.638e-15	-14.036	-14.117	-0.081	(0)
Cd(OH)3-	5.305e-18	4.403e-18	-17.275	-17.356	-0.081	(0)
Cd2OH+3	2.394e-18	4.726e-19	-17.621	-18.326	-0.705	(0)
Cd(OH)4-2	1.222e-23	5.732e-24	-22.913	-23.242	-0.329	(0)
Cd4(OH)4+4	0.000e+00	0.000e+00	-362.465	-363.688	-1.223	(0)
Cl(-1)	2.060e-03					
Cl-	2.054e-03	1.687e-03	-2.687	-2.773	-0.086	(0)
NaCl	5.510e-06	5.510e-06	-5.259	-5.259	0.000	(0)
CaCl+	4.799e-07	3.983e-07	-6.319	-6.400	-0.081	(0)
MgCl+	1.804e-07	1.498e-07	-6.744	-6.825	-0.081	(0)
KCl	4.579e-09	4.579e-09	-8.339	-8.339	0.000	(0)
CdCl+	2.909e-09	2.415e-09	-8.536	-8.617	-0.081	(0)
CaCl2	7.901e-10	7.901e-10	-9.102	-9.102	0.000	(0)
CuCl2-	3.574e-11	2.967e-11	-10.447	-10.528	-0.081	(0)
Cd(OH)Cl	2.534e-11	2.534e-11	-10.596	-10.596	0.000	(0)
CdCl2	1.766e-11	1.766e-11	-10.753	-10.753	0.000	(0)
CuCl+	1.598e-11	1.327e-11	-10.796	-10.877	-0.081	(0)
HCl	2.621e-12	2.621e-12	-11.582	-11.582	0.000	(0)
CuCl3-2	6.852e-13	3.213e-13	-12.164	-12.493	-0.329	(0)
FeCl+	1.038e-13	8.616e-14	-12.984	-13.065	-0.081	(0)
CuCl2	1.178e-14	1.178e-14	-13.929	-13.929	0.000	(0)
CdCl3-	9.203e-15	7.638e-15	-14.036	-14.117	-0.081	(0)
FeCl2	7.798e-19	7.798e-19	-18.108	-18.108	0.000	(0)
FeCl+2	3.951e-23	1.889e-23	-22.403	-22.724	-0.320	(0)
FeCl2+	3.108e-23	2.580e-23	-22.507	-22.588	-0.081	(0)
FeCl4-2	1.367e-23	6.409e-24	-22.864	-23.193	-0.329	(0)
CuCl4-2	1.341e-24	6.289e-25	-23.872	-24.201	-0.329	(0)
FeCl4-	1.063e-31	8.822e-32	-30.973	-31.054	-0.081	(0)
Cl(1)	4.008e-37					
ClO-	3.304e-37	2.743e-37	-36.481	-36.562	-0.081	(0)
HClO	7.037e-38	7.037e-38	-37.153	-37.153	0.000	(0)
Cl(3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-63.164	-63.245	-0.081	(0)
HClO2	0.000e+00	0.000e+00	-68.235	-68.235	0.000	(0)
Cl(5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-75.993	-76.076	-0.083	(0)
Cl(7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-93.126	-93.209	-0.083	(0)
Cu(1)	2.261e-10					
Cu+	1.897e-10	1.574e-10	-9.722	-9.803	-0.081	(0)

CuCl2-	3.574e-11	2.967e-11	-10.447	-10.528	-0.081 (0)
CuCl3-2	6.852e-13	3.213e-13	-12.164	-12.493	-0.329 (0)
Cu(2)	2.048e-07				
CuCO3	1.660e-07	1.660e-07	-6.780	-6.780	0.000 (0)
CuOH+	2.581e-08	2.142e-08	-7.588	-7.669	-0.081 (0)
Cu+2	5.700e-09	2.876e-09	-8.244	-8.541	-0.297 (0)
Cu(CO3)2-2	3.816e-09	1.789e-09	-8.418	-8.747	-0.329 (0)
CuSO4	3.389e-09	3.389e-09	-8.470	-8.470	0.000 (0)
CuCO3(OH)2-2	6.278e-11	2.944e-11	-10.202	-10.531	-0.329 (0)
CuCl+	1.598e-11	1.327e-11	-10.796	-10.877	-0.081 (0)
CuNO2+	1.279e-12	1.061e-12	-11.893	-11.974	-0.081 (0)
CuF+	1.177e-12	9.769e-13	-11.929	-12.010	-0.081 (0)
CuCl2	1.178e-14	1.178e-14	-13.929	-13.929	0.000 (0)
CuO2-2	9.490e-16	4.450e-16	-15.023	-15.352	-0.329 (0)
Cu(NO2)2	3.829e-17	3.829e-17	-16.417	-16.417	0.000 (0)
CuCl4-2	1.341e-24	6.289e-25	-23.872	-24.201	-0.329 (0)
F	2.690e-05				
F-	2.596e-05	2.143e-05	-4.586	-4.669	-0.083 (0)
AsO3F-2	6.802e-07	3.189e-07	-6.167	-6.496	-0.329 (0)
CaF+	1.463e-07	1.214e-07	-6.835	-6.916	-0.081 (0)
MgF+	7.089e-08	5.883e-08	-7.149	-7.230	-0.081 (0)
NaF	4.261e-08	4.261e-08	-7.370	-7.370	0.000 (0)
HAsO3F-	1.974e-09	1.638e-09	-8.705	-8.786	-0.081 (0)
HF	2.276e-10	2.276e-10	-9.643	-9.643	0.000 (0)
CuF+	1.177e-12	9.769e-13	-11.929	-12.010	-0.081 (0)
AlF2+	3.299e-13	2.738e-13	-12.482	-12.562	-0.081 (0)
AlF3	7.389e-14	7.389e-14	-13.131	-13.131	0.000 (0)
AlF+2	6.711e-14	3.209e-14	-13.173	-13.494	-0.320 (0)
FeF+	4.149e-14	3.443e-14	-13.382	-13.463	-0.081 (0)
HF2-	1.424e-15	1.182e-15	-14.847	-14.927	-0.081 (0)
BF2(OH)2-	1.183e-15	9.822e-16	-14.927	-15.008	-0.081 (0)
AlF4-	4.793e-16	3.978e-16	-15.319	-15.400	-0.081 (0)
H2F2	1.289e-19	1.289e-19	-18.890	-18.890	0.000 (0)
FeF+2	4.519e-20	2.161e-20	-19.345	-19.665	-0.320 (0)
FeF2+	9.031e-21	7.496e-21	-20.044	-20.125	-0.081 (0)
BF3OH-	7.491e-22	6.217e-22	-21.125	-21.206	-0.081 (0)
BF4-	7.368e-30	6.115e-30	-29.133	-29.214	-0.081 (0)
Fe(2)	2.661e-10				
Fe+2	1.390e-10	7.013e-11	-9.857	-10.154	-0.297 (0)
FeSO4	5.718e-11	5.718e-11	-10.243	-10.243	0.000 (0)
FeHCO3+	4.184e-11	3.473e-11	-10.378	-10.459	-0.081 (0)
FeCO3	2.409e-11	2.409e-11	-10.618	-10.618	0.000 (0)
FeOH+	3.859e-12	3.203e-12	-11.414	-11.494	-0.081 (0)
FeCl+	1.038e-13	8.616e-14	-12.984	-13.065	-0.081 (0)
FeF+	4.149e-14	3.443e-14	-13.382	-13.463	-0.081 (0)
Fe(OH)2	3.675e-15	3.675e-15	-14.435	-14.435	0.000 (0)
Fe(OH)3-	2.546e-17	2.113e-17	-16.594	-16.675	-0.081 (0)
FeCl2	7.798e-19	7.798e-19	-18.108	-18.108	0.000 (0)
FeCl4-2	1.367e-23	6.409e-24	-22.864	-23.193	-0.329 (0)
Fe(OH)4-2	6.508e-24	3.052e-24	-23.187	-23.515	-0.329 (0)
Fe(3)	2.151e-07				
Fe(OH)3	2.026e-07	2.026e-07	-6.693	-6.693	0.000 (0)
Fe(OH)4-	8.855e-09	7.350e-09	-8.053	-8.134	-0.081 (0)
Fe(OH)2+	3.613e-09	2.999e-09	-8.442	-8.523	-0.081 (0)
FeOH+2	1.311e-13	6.270e-14	-12.882	-13.203	-0.320 (0)
FeCO3+	2.831e-15	2.350e-15	-14.548	-14.629	-0.081 (0)
Fe+3	2.592e-19	6.724e-20	-18.586	-19.172	-0.586 (0)
FeF+2	4.519e-20	2.161e-20	-19.345	-19.665	-0.320 (0)
FeSO4+	4.032e-20	3.347e-20	-19.394	-19.475	-0.081 (0)
FeF2+	9.031e-21	7.496e-21	-20.044	-20.125	-0.081 (0)
FeNO3+2	4.751e-21	2.272e-21	-20.323	-20.644	-0.320 (0)
Fe(SO4)2-	3.507e-21	2.911e-21	-20.455	-20.536	-0.081 (0)
FeNO2+2	7.000e-22	3.348e-22	-21.155	-21.475	-0.320 (0)
FeCl+2	3.951e-23	1.889e-23	-22.403	-22.724	-0.320 (0)
FeCl2+	3.108e-23	2.580e-23	-22.507	-22.588	-0.081 (0)
Fe2(OH)2+4	1.769e-24	1.058e-25	-23.752	-24.975	-1.223 (0)
Fe3(OH)4+5	4.872e-30	6.630e-32	-29.312	-31.178	-1.866 (0)

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  FeCl4-          1.063e-31   8.822e-32   -30.973   -31.054    -0.081     (0)
H(0)          7.519e-28
  H2              3.759e-28   3.798e-28   -27.425   -27.420     0.004     (0)
K             1.025e-04
  K+              9.847e-05   8.086e-05    -4.007    -4.092    -0.086     (0)
  KSO4-           4.045e-06   3.358e-06    -5.393    -5.474    -0.081     (0)
  KCl             4.579e-09   4.579e-09    -8.339    -8.339     0.000     (0)
  KOH             4.049e-11   4.049e-11   -10.393   -10.393     0.000     (0)
  KHSO4           2.050e-14   2.050e-14   -13.688   -13.688     0.000     (0)
Mg            3.711e-04
  Mg+2            2.123e-04   1.137e-04    -3.673    -3.944    -0.271     (0)
  MgSO4           1.563e-04   1.563e-04    -3.806    -3.806     0.000     (0)
  MgHCO3+         1.502e-06   1.247e-06    -5.823    -5.904    -0.081     (0)
  MgCO3           7.281e-07   7.281e-07    -6.138    -6.138     0.000     (0)
  MgCl+           1.804e-07   1.498e-07    -6.744    -6.825    -0.081     (0)
  MgF+            7.089e-08   5.883e-08    -7.149    -7.230    -0.081     (0)
  MgB(OH)4+       6.639e-08   5.510e-08    -7.178    -7.259    -0.081     (0)
  Mg4(OH)4+4      2.165e-22   1.295e-23   -21.664   -22.888    -1.223     (0)
N(3)          4.293e-06
  NO2-            4.293e-06   3.525e-06    -5.367    -5.453    -0.086     (0)
  HNO2            4.162e-11   4.162e-11   -10.381   -10.381     0.000     (0)
  CdNO2+          2.806e-12   2.329e-12   -11.552   -11.633    -0.081     (0)
  CuNO2+          1.279e-12   1.061e-12   -11.893   -11.974    -0.081     (0)
  Cu(NO2)2        3.829e-17   3.829e-17   -16.417   -16.417     0.000     (0)
  FeNO2+2         7.000e-22   3.348e-22   -21.155   -21.475    -0.320     (0)
N(5)          4.138e-03
  NO3-            4.115e-03   3.379e-03    -2.386    -2.471    -0.086     (0)
  CaNO3+          2.274e-05   1.887e-05    -4.643    -4.724    -0.081     (0)
  HNO3            1.223e-12   1.223e-12   -11.913   -11.913     0.000     (0)
  FeNO3+2         4.751e-21   2.272e-21   -20.323   -20.644    -0.320     (0)
Na            2.319e-02
  Na+             2.240e-02   1.859e-02    -1.650    -1.731    -0.081     (0)
  NaSO4-          7.613e-04   6.318e-04    -3.118    -3.199    -0.081     (0)
  NaHCO3          2.509e-05   2.509e-05    -4.601    -4.601     0.000     (0)
  NaCl            5.510e-06   5.510e-06    -5.259    -5.259     0.000     (0)
  NaCO3-          4.742e-07   3.936e-07    -6.324    -6.405    -0.081     (0)
  NaB(OH)4        2.124e-07   2.124e-07    -6.673    -6.673     0.000     (0)
  NaF             4.261e-08   4.261e-08    -7.370    -7.370     0.000     (0)
  NaOH            4.463e-09   4.463e-09    -8.350    -8.350     0.000     (0)
  NaAlO2          3.001e-09   3.001e-09    -8.523    -8.523     0.000     (0)
O(0)          8.727e-38
  O2              4.363e-38   4.408e-38   -37.360   -37.356     0.004     (0)
S(6)          1.273e-02
  SO4-2           1.097e-02   5.145e-03    -1.960    -2.289    -0.329     (0)
  CaSO4           8.373e-04   8.373e-04    -3.077    -3.077     0.000     (0)
  NaSO4-          7.613e-04   6.318e-04    -3.118    -3.199    -0.081     (0)
  MgSO4           1.563e-04   1.563e-04    -3.806    -3.806     0.000     (0)
  KSO4-           4.045e-06   3.358e-06    -5.393    -5.474    -0.081     (0)
  HSO4-           4.332e-09   3.595e-09    -8.363    -8.444    -0.081     (0)
  CuSO4           3.389e-09   3.389e-09    -8.470    -8.470     0.000     (0)
  FeSO4           5.718e-11   5.718e-11   -10.243   -10.243     0.000     (0)
  CdSO4           1.471e-11   1.471e-11   -10.832   -10.832     0.000     (0)
  KHSO4           2.050e-14   2.050e-14   -13.688   -13.688     0.000     (0)
  AlSO4+          9.498e-16   7.883e-16   -15.022   -15.103    -0.081     (0)
  Al(SO4)2-       3.793e-16   3.148e-16   -15.421   -15.502    -0.081     (0)
  FeSO4+          4.032e-20   3.347e-20   -19.394   -19.475    -0.081     (0)
  H2SO4           2.347e-20   2.347e-20   -19.630   -19.630     0.000     (0)
  Fe(SO4)2-       3.507e-21   2.911e-21   -20.455   -20.536    -0.081     (0)

-------------------------------Saturation indices--------------------------------

  Phase               SI** log IAP   log K(298 K,   1 atm)

  Al             -113.24     36.67  149.91  Al
  Al(g)          -163.95     36.67  200.62  Al
  Al2(SO4)3       -57.41    -38.52   18.90  Al2(SO4)3
  Al2(SO4)3:6H2O  -40.07    -38.52    1.56  Al2(SO4)3:6H2O
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AlF3	-12.57	-29.83	-17.27 AlF3
Alum-K	-19.53	-24.50	-4.97 KAl(SO4)2:12H2O
Alunite	-6.72	-7.19	-0.47 KAl3(OH)6(SO4)2
Anhydrite	-0.89	-5.24	-4.35 CaSO4
Antarcticite	-12.59	-8.50	4.09 CaCl2:6H2O
Antlerite	-4.00	4.73	8.73 Cu3(SO4)(OH)4
Aphthitalite	-14.70	-18.58	-3.89 NaK3(SO4)2
Aragonite	0.21	2.18	1.97 CaCO3
Arcanite	-8.63	-10.47	-1.84 K2SO4
Arsenolite	-104.33	-124.17	-19.84 As2O3
Artinite	-6.06	13.56	19.63 Mg2CO3(OH)2:3H2O
As	-76.75	-34.07	42.68 As
As2O5	-102.60	-100.46	2.14 As2O5
As4O6(cubi)	-208.52	-248.35	-39.82 As4O6
As4O6(mono)	-208.30	-248.35	-40.05 As4O6
Atacamite	-5.02	9.25	14.26 Cu4Cl2(OH)6
Azurite	-8.15	0.97	9.12 Cu3(CO3)2(OH)2
B	-85.67	23.89	109.56 B
B(g)	-176.95	23.89	200.84 B
B2O3	-13.80	-8.25	5.55 B2O3
Bassanite	-1.54	-5.24	-3.71 CaSO4:0.5H2O
BF3(g)	-39.63	-42.61	-2.98 BF3
Bischofite	-13.88	-9.49	4.39 MgCl2:6H2O
Bloedite	-9.51	-11.98	-2.48 Na2Mg(SO4)2:4H2O
Boehmite	1.11	8.65	7.55 AlO2H
Borax	-15.70	-3.65	12.04 Na2(B4O5(OH)4):8H2O
Boric_acid	-3.97	-4.13	-0.16 B(OH)3
Brochantite	-2.92	12.50	15.42 Cu4(SO4)(OH)6
Brucite	-3.91	12.38	16.28 Mg(OH)2
Burkeite	-19.31	-9.83	9.49 Na6CO3(SO4)2
C	-37.98	26.17	64.15 C
C(g)	-155.59	26.17	181.77 C
Ca	-107.79	32.04	139.83 Ca
Ca(g)	-133.03	32.04	165.07 Ca
Ca2Al2O5:8H2O	-15.53	44.04	59.57 Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-21.42	4.87	26.29 Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-78.17	-60.36	17.80 Ca3(AsO4)2
Ca3Al2O6	-55.62	57.41	113.03 Ca3Al2O6
Ca4Al2Fe2O10	-59.09	81.39	140.48 Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-36.48	70.77	107.25 Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-32.91	70.77	103.68 Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-36.73	31.60	68.33 Ca4Cl2(OH)6:13H2O
CaAl2O4	-16.23	30.68	46.91 CaAl2O4
CaAl2O4:10H2O	-7.32	30.67	37.99 CaAl2O4:10H2O
CaAl4O7	-20.61	47.99	68.59 CaAl4O7
Calcite	0.36	2.18	1.82 CaCO3
Carnallite	-20.63	-16.36	4.27 KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.71	-5.24	-3.54 CaSO4:0.5H2O
Cd	-30.14	26.45	56.59 Cd
Cd(BO2)2	-10.31	-0.48	9.83 Cd(BO2)2
Cd(g)	-43.68	26.45	70.13 Cd
Cd(OH)2	-5.97	7.77	13.73 Cd(OH)2
Cd(OH)Cl	-6.70	-3.16	3.54 Cd(OH)Cl
Cd3(AsO4)2	-81.22	-77.16	4.06 Cd3(AsO4)2
Cd3(SO4)(OH)4	-17.87	4.70	22.57 Cd3(SO4)(OH)4
Cd3(SO4)2(OH)2	-20.63	-13.91	6.72 Cd3(SO4)2(OH)2
CdCl2	-13.44	-14.10	-0.66 CdCl2
CdCl2:H2O	-12.41	-14.10	-1.68 CdCl2:H2O
CdF2	-16.73	-17.89	-1.16 CdF2
CdSO4	-10.72	-10.84	-0.12 CdSO4
CdSO4:2.667H2O	-9.03	-10.84	-1.81 CdSO4:2.667H2O
CdSO4:H2O	-9.17	-10.84	-1.66 CdSO4:H2O
Chalcanthite	-8.20	-10.83	-2.63 CuSO4:5H2O
Chalcocyanite	-13.74	-10.83	2.91 CuSO4
Chloromagnesite	-31.31	-9.49	21.82 MgCl2
Cl2(g)	-43.54	-40.54	2.99 Cl2
Claudetite	-104.38	-124.17	-19.80 As2O3

CO2(g)	-3.36	-11.18	-7.83 CO2
Colemanite	-19.55	1.97	21.51 Ca2B6O11:5H2O
Corundum	-0.98	17.31	18.29 Al2O3
Cu	-5.04	26.46	31.50 Cu
Cu(g)	-57.20	26.46	83.66 Cu
CuCl2	-17.81	-14.09	3.72 CuCl2
CuF	-21.55	-14.47	7.08 CuF
CuF2	-17.26	-17.88	-0.62 CuF2
CuF2:2H2O	-13.33	-17.88	-4.55 CuF2:2H2O
Cuprite	-1.38	-3.29	-1.91 Cu2O
Dawsonite	-0.44	3.90	4.34 NaAlCO3(OH)2
Delafossite	10.10	3.66	-6.44 CuFeO2
Diaspore	1.51	8.65	7.15 AlHO2
Dolomite	0.90	3.37	2.47 CaMg(CO3)2
Dolomite-dis	-0.64	3.37	4.01 CaMg(CO3)2
Dolomite-ord	0.91	3.37	2.46 CaMg(CO3)2
Epsomite	-4.27	-6.24	-1.96 MgSO4:7H2O
Ettringite	-20.79	41.67	62.46 Ca6Al2(SO4)3(OH)12:26H2O
F2(g)	-100.05	-44.34	55.71 F2
Fe	-34.17	24.84	59.02 Fe
Fe(OH)2	-7.73	6.17	13.89 Fe(OH)2
Fe(OH)3	-0.33	5.31	5.64 Fe(OH)3
Fe2(SO4)3	-48.26	-45.21	3.05 Fe2(SO4)3
FeF2	-17.07	-19.49	-2.42 FeF2
FeF3	-13.92	-33.18	-19.26 FeF3
FeO	-7.36	6.17	13.52 FeO
Ferrite-Ca	2.49	23.98	21.50 CaFe2O4
Ferrite-Cu	8.11	18.39	10.28 CuFe2O4
Ferrite-Dicalcium	-19.45	37.35	56.80 Ca2Fe2O5
Ferrite-Mg	1.97	22.99	21.02 MgFe2O4
FeSO4	-15.05	-12.44	2.61 FeSO4
Fluorite	-2.22	-12.29	-10.07 CaF2
Gaylussite	-7.31	3.85	11.16 CaNa2(CO3)2:5H2O
Gibbsite	0.91	8.65	7.74 Al(OH)3
Glauberite	-5.52	-10.99	-5.47 Na2Ca(SO4)2
Goethite	4.78	5.31	0.53 FeOOH
Gypsum	-0.71	-5.24	-4.53 CaSO4:2H2O
H2(g)	-24.32	-27.42	-3.10 H2
H2O(g)	-1.59	-0.00	1.59 H2O
Halite	-6.07	-4.50	1.56 NaCl
HCl(g)	-17.23	-10.93	6.30 HCl
Hematite	10.54	10.61	0.08 Fe2O3
Hercynite	-5.33	23.48	28.80 FeAl2O4
Hexahydrite	-4.51	-6.23	-1.73 MgSO4:6H2O
Huntite	-4.46	5.75	10.22 CaMg3(CO3)4
Hydroboracite	-19.39	0.98	20.36 MgCaB6O11:6H2O
Hydromagnesite	-13.60	17.14	30.74 Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-20.24	-8.50	11.75 CaCl2
Ice	-0.14	-0.00	0.14 H2O
Jarosite	-7.82	-17.23	-9.41 KFe3(SO4)2(OH)6
Jarosite-Na	-9.42	-14.87	-5.45 NaFe3(SO4)2(OH)6
K	-57.57	13.41	70.98 K
K(g)	-68.17	13.41	81.58 K
K2CO3:1.5H2O	-16.43	-3.05	13.38 K2CO3:1.5H2O
K2O	-75.90	8.14	84.04 K2O
K3H(SO4)2	-21.39	-25.01	-3.62 K3H(SO4)2
K8H4(CO3)6:3H2O	-62.28	-34.57	27.71 K8H4(CO3)6:3H2O
Kainite	-12.79	-13.10	-0.31 KMgClSO4:3H2O
KAl(SO4)2	-27.77	-24.49	3.27 KAl(SO4)2
Kalicinite	-7.40	-7.12	0.28 KHCO3
Katoite	-21.54	57.41	78.94 Ca3Al2H12O12
Kieserite	-5.97	-6.23	-0.27 MgSO4:H2O
KMgCl3	-37.60	-16.36	21.25 KMgCl3
KMgCl3:2H2O	-30.32	-16.36	13.96 KMgCl3:2H2O
KNaCO3:6H2O	-10.95	-0.69	10.26 KNaCO3:6H2O
Lammerite	-78.68	-77.13	1.55 Cu3(AsO4)2
Lansfordite	-3.65	1.19	4.84 MgCO3:5H2O

Lawrencite	-24.75	-15.70	9.05 FeCl2
Leonite	-12.59	-16.71	-4.11 K2Mg(SO4)2:4H2O
Lime	-19.20	13.37	32.57 CaO
Magnesite	-1.08	1.19	2.27 MgCO3
Magnetite	6.36	16.78	10.42 Fe3O4
Malachite	-1.53	4.37	5.90 Cu2CO3(OH)2
Mayenite	-212.58	281.57	494.15 Ca12Al14O33
Melanterite	-10.05	-12.45	-2.40 FeSO4:7H2O
Mercallite	-13.10	-14.54	-1.44 KHSO4
Mg	-91.47	31.05	122.52 Mg
Mg(g)	-111.19	31.05	142.25 Mg
Mg1.25SO4(OH)0.5:0.5H2O	-8.33	-3.14	5.20 Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-9.25	-0.05	9.21 Mg1.5SO4(OH)
MgCl2:2H2O	-22.22	-9.49	12.73 MgCl2:2H2O
MgCl2:4H2O	-16.79	-9.49	7.30 MgCl2:4H2O
MgCl2:H2O	-25.56	-9.49	16.07 MgCl2:H2O
MgOHCl	-14.45	1.44	15.89 MgOHCl
MgSO4	-11.06	-6.23	4.83 MgSO4
Mirabilite	-4.60	-5.75	-1.15 Na2SO4:10H2O
Misenite	-86.64	-97.72	-11.08 K8H6(SO4)7
Molysite	-40.96	-27.49	13.47 FeCl3
Monohydrocalcite	-0.50	2.18	2.68 CaCO3:H2O
Monteponite	-7.32	7.77	15.09 CdO
Na	-51.60	15.77	67.37 Na
Na(g)	-65.09	15.77	80.86 Na
Na2CO3	-9.49	1.67	11.16 Na2CO3
Na2CO3:7H2O	-8.27	1.67	9.94 Na2CO3:7H2O
Na2O	-54.56	12.86	67.42 Na2O
Na3H(SO4)2	-17.04	-17.93	-0.89 Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-10.85	-16.74	-5.89 Na4Ca(SO4)3:2H2O
NaFeO2	-8.15	11.74	19.88 NaFeO2
Nahcolite	-4.61	-4.76	-0.14 NaHCO3
Nantokite	-5.81	-12.58	-6.77 CuCl
Natron	-7.92	1.67	9.59 Na2CO3:10H2O
Nesquehonite	-4.10	1.19	5.29 MgCO3:3H2O
Niter	-6.34	-6.56	-0.22 KNO3
NO(g)	-5.01	-4.27	0.74 NO
NO2(g)	-9.64	-1.29	8.35 NO2
O2(g)	-34.46	-37.36	-2.89 O2
Otavite	-1.64	-3.42	-1.77 CdCO3
Oxychloride-Mg	-12.02	13.82	25.83 Mg2Cl(OH)3:4H2O
Pentahydrite	-4.85	-6.23	-1.39 MgSO4:5H2O
Periclase	-8.95	12.38	21.33 MgO
Picromerite	-12.27	-16.71	-4.44 K2Mg(SO4)2:6H2O
Pirssonite	-7.47	3.85	11.32 Na2Ca(CO3)2:2H2O
Polyhalite	-12.88	-27.19	-14.31 K2MgCa2(SO4)4:2H2O
Portlandite	-9.18	13.37	22.55 Ca(OH)2
Sellaite	-3.84	-13.28	-9.44 MgF2
Siderite	-4.80	-5.02	-0.22 FeCO3
Spinel	-7.92	29.69	37.61 Al2MgO4
Starkeyite	-5.23	-6.23	-1.00 MgSO4:4H2O
Sylvite	-7.69	-6.87	0.83 KCl
Syngenite	-8.12	-15.72	-7.60 K2Ca(SO4)2:H2O
Tachyhydrite	-44.63	-27.48	17.14 Mg2CaCl6:12H2O
Tenorite	0.13	7.78	7.65 CuO
Thenardite	-5.39	-5.75	-0.36 Na2SO4
Thermonatrite	-9.26	1.67	10.94 Na2CO3:H2O
Trona-K	-19.40	-7.81	11.59 K2NaH(CO3)2:2H2O
Wustite	-6.66	5.75	12.40 Fe.947O

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 4.

```
SOLUTION 2 WKQ_HBh2
   temp      25
   pH        7.36
   pe        4
   redox     pe
   units     mg/l
   density   1
   Al        11 ug/l
   Alkalinity 312.4
   B         103 ug/l
   Ba        25 ug/l
   Ca        71
   Cl        19.99
   Cu        24 ug/l
   F         0.43
   Fe        244 ug/l
   K         1
   Mg        39
   Mn        5
   N(5)      5.08 as N
   Na        23
   S(6)      63.01 as SO4-2
   Zn        0.04
   water     1 # kg
END
```

Beginning of initial solution calculations.

Initial solution 2. WKQ_HBh2

----------Solution composition----------

Elements	Molality	Moles
Al	4.079e-07	4.079e-07
Alkalinity	6.247e-03	6.247e-03
B	9.532e-06	9.532e-06
Ba	1.821e-07	1.821e-07
Ca	1.773e-03	1.773e-03
Cl	5.642e-04	5.642e-04
Cu	3.779e-07	3.779e-07
F	2.265e-05	2.265e-05
Fe	4.371e-06	4.371e-06
K	2.559e-05	2.559e-05
Mg	1.605e-03	1.605e-03
Mn	9.106e-05	9.106e-05
N(5)	3.629e-04	3.629e-04
Na	1.001e-03	1.001e-03
S(6)	6.564e-04	6.564e-04
Zn	6.120e-07	6.120e-07

----------Description of solution----------

```
                        pH  =   7.360
                        pe  =   4.000
          Activity of water  =   1.000
Ionic strength (mol/kgw)  =   1.140e-02
     Mass of water (kg)  =   1.000e+00
  Total carbon (mol/kg)  =   6.749e-03
    Total CO2 (mol/kg)  =   6.749e-03
       Temperature (°C)  =  25.00
 Electrical balance (eq)  =  -5.356e-04
```

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -3.46
                        Iterations  =  7
                          Total H  = 1.110569e+02
                          Total O  = 5.554878e+01

----------------------------Distribution of species----------------------------

                                    Log      Log      Log    mole V
  Species          Molality    Activity Molality Activity    Gamma   cm³/mol

  OH-             2.466e-07   2.207e-07   -6.608   -6.656   -0.048     (0)
  H+              4.798e-08   4.365e-08   -7.319   -7.360   -0.041     0.00
  H2O             5.553e+01   9.998e-01    1.744   -0.000    0.000    18.07
Al             4.079e-07
  AlO2-           3.646e-07   3.268e-07   -6.438   -6.486   -0.047     (0)
  HAlO2           4.165e-08   4.165e-08   -7.380   -7.380    0.000     (0)
  Al(OH)2+        1.393e-09   1.249e-09   -8.856   -8.903   -0.047     (0)
  AlF2+           1.573e-10   1.410e-10   -9.803   -9.851   -0.047     (0)
  NaAlO2          5.545e-11   5.545e-11  -10.256  -10.256    0.000     (0)
  AlOH+2          3.623e-11   2.349e-11  -10.441  -10.629   -0.188     (0)
  AlF3            3.491e-11   3.491e-11  -10.457  -10.457    0.000     (0)
  AlF+2           2.777e-11   1.801e-11  -10.556  -10.745   -0.188     (0)
  Al+3            2.161e-13   9.155e-14  -12.665  -13.038   -0.373     (0)
  AlF4-           1.924e-13   1.725e-13  -12.716  -12.763   -0.047     (0)
  AlSO4+          3.447e-14   3.091e-14  -13.463  -13.510   -0.047     (0)
  Al(SO4)2-       8.828e-16   7.914e-16  -15.054  -15.102   -0.047     (0)
  Al2(OH)2+4      4.839e-19   8.972e-20  -18.315  -19.047   -0.732     (0)
  Al3(OH)4+5      3.728e-23   2.781e-24  -22.428  -23.556   -1.127     (0)
  Al13O4(OH)24+7  3.152e-31   1.944e-33  -30.501  -32.711   -2.210     (0)
B(-5)          0.000e+00
  BH4-            0.000e+00   0.000e+00 -153.594 -153.642   -0.047     (0)
B(3)           9.532e-06
  B(OH)3          9.383e-06   9.383e-06   -5.028   -5.028    0.000     (0)
  BO2-            1.286e-07   1.153e-07   -6.891   -6.938   -0.047     (0)
  MgB(OH)4+       1.054e-08   9.446e-09   -7.977   -8.025   -0.047     (0)
  CaB(OH)4+       9.755e-09   8.746e-09   -8.011   -8.058   -0.047     (0)
  NaB(OH)4        2.029e-10   2.029e-10   -9.693   -9.693    0.000     (0)
  BaB(OH)4+       4.487e-13   4.023e-13  -12.348  -12.395   -0.047     (0)
  BF2(OH)2-       7.325e-16   6.567e-16  -15.135  -15.183   -0.047     (0)
  BF3OH-          2.683e-21   2.406e-21  -20.571  -20.619   -0.047     (0)
  B2O(OH)5-       4.646e-22   4.165e-22  -21.333  -21.380   -0.047     (0)
  BF4-            1.527e-28   1.369e-28  -27.816  -27.864   -0.047     (0)
Ba             1.821e-07
  Ba+2            1.815e-07   1.184e-07   -6.741   -6.927   -0.185     (0)
  BaNO3+          3.383e-10   3.033e-10   -9.471   -9.518   -0.047     (0)
  BaCO3           3.169e-10   3.169e-10   -9.499   -9.499    0.000     (0)
  BaCl+           2.231e-11   2.000e-11  -10.652  -10.699   -0.047     (0)
  BaF+            1.790e-12   1.605e-12  -11.747  -11.795   -0.047     (0)
  BaB(OH)4+       4.487e-13   4.023e-13  -12.348  -12.395   -0.047     (0)
  BaOH+           1.025e-13   9.191e-14  -12.989  -13.037   -0.047     (0)
C(4)           6.749e-03
  HCO3-           6.012e-03   5.390e-03   -2.221   -2.268   -0.047     (0)
  CO2             5.443e-04   5.459e-04   -3.264   -3.263    0.001     (0)
  CaHCO3+         7.664e-05   6.871e-05   -4.116   -4.163   -0.047     (0)
  MgHCO3+         6.818e-05   6.113e-05   -4.166   -4.214   -0.047     (0)
  CaCO3           1.366e-05   1.366e-05   -4.865   -4.865    0.000     (0)
  MnCO3           9.514e-06   9.514e-06   -5.022   -5.022    0.000     (0)
  CO3-2           8.449e-06   5.478e-06   -5.073   -5.261   -0.188     (0)
  NaHCO3          6.856e-06   6.856e-06   -5.164   -5.164    0.000     (0)
  MgCO3           5.659e-06   5.659e-06   -5.247   -5.247    0.000     (0)
  MnHCO3+         2.271e-06   2.036e-06   -5.644   -5.691   -0.047     (0)
  FeHCO3+         7.734e-07   6.934e-07   -6.112   -6.159   -0.047     (0)
  CuCO3           3.525e-07   3.525e-07   -6.453   -6.453    0.000     (0)
  FeCO3           7.624e-08   7.624e-08   -7.118   -7.118    0.000     (0)
  ZnHCO3+         5.223e-08   4.683e-08   -7.282   -7.329   -0.047     (0)
  NaCO3-          1.901e-08   1.704e-08   -7.721   -7.768   -0.047     (0)
  ZnCO3           1.551e-08   1.551e-08   -7.810   -7.810    0.000     (0)
```

Cu(CO3)2-2	5.341e-09	3.440e-09	-8.272	-8.463	-0.191	(0)
BaCO3	3.169e-10	3.169e-10	-9.499	-9.499	0.000	(0)
FeCO3+	8.293e-12	7.435e-12	-11.081	-11.129	-0.047	(0)
CuCO3(OH)2-2	2.441e-12	1.572e-12	-11.612	-11.804	-0.191	(0)
Ca	1.773e-03					
Ca+2	1.628e-03	1.076e-03	-2.788	-2.968	-0.180	(0)
CaHCO3+	7.664e-05	6.871e-05	-4.116	-4.163	-0.047	(0)
CaSO4	5.184e-05	5.184e-05	-4.285	-4.285	0.000	(0)
CaCO3	1.366e-05	1.366e-05	-4.865	-4.865	0.000	(0)
CaNO3+	1.939e-06	1.739e-06	-5.712	-5.760	-0.047	(0)
CaCl+	1.280e-07	1.148e-07	-6.893	-6.940	-0.047	(0)
CaF+	1.200e-07	1.076e-07	-6.921	-6.968	-0.047	(0)
CaB(OH)4+	9.755e-09	8.746e-09	-8.011	-8.058	-0.047	(0)
CaOH+	3.882e-09	3.480e-09	-8.411	-8.458	-0.047	(0)
CaCl2	6.797e-11	6.797e-11	-10.168	-10.168	0.000	(0)
Cl(-1)	5.642e-04					
Cl-	5.635e-04	5.034e-04	-3.249	-3.298	-0.049	(0)
MgCl+	4.281e-07	3.838e-07	-6.368	-6.416	-0.047	(0)
CaCl+	1.280e-07	1.148e-07	-6.893	-6.940	-0.047	(0)
NaCl	7.868e-08	7.868e-08	-7.104	-7.104	0.000	(0)
MnCl+	5.932e-08	5.318e-08	-7.227	-7.274	-0.047	(0)
KCl	3.855e-10	3.855e-10	-9.414	-9.414	0.000	(0)
ZnCl+	3.180e-10	2.851e-10	-9.498	-9.545	-0.047	(0)
Zn(OH)Cl	1.116e-10	1.116e-10	-9.952	-9.952	0.000	(0)
FeCl+	1.003e-10	8.989e-11	-9.999	-10.046	-0.047	(0)
CaCl2	6.797e-11	6.797e-11	-10.168	-10.168	0.000	(0)
BaCl+	2.231e-11	2.000e-11	-10.652	-10.699	-0.047	(0)
CuCl+	1.036e-11	9.290e-12	-10.985	-11.032	-0.047	(0)
CuCl2-	6.916e-12	6.201e-12	-11.160	-11.208	-0.047	(0)
HCl	4.936e-12	4.936e-12	-11.307	-11.307	0.000	(0)
ZnCl2	1.676e-13	1.676e-13	-12.776	-12.776	0.000	(0)
CuCl3-2	3.113e-14	2.005e-14	-13.507	-13.698	-0.191	(0)
MnCl3-	3.284e-15	2.944e-15	-14.484	-14.531	-0.047	(0)
CuCl2	2.463e-15	2.463e-15	-14.609	-14.609	0.000	(0)
FeCl2	2.428e-16	2.428e-16	-15.615	-15.615	0.000	(0)
ZnCl3-	5.198e-17	4.661e-17	-16.284	-16.332	-0.047	(0)
ZnCl4-2	2.761e-19	1.778e-19	-18.559	-18.750	-0.191	(0)
FeCl+2	3.040e-20	1.971e-20	-19.517	-19.705	-0.188	(0)
FeCl2+	8.961e-21	8.034e-21	-20.048	-20.095	-0.047	(0)
FeCl4-2	2.761e-22	1.778e-22	-21.559	-21.750	-0.191	(0)
CuCl4-2	1.819e-26	1.171e-26	-25.740	-25.931	-0.191	(0)
FeCl4-	2.730e-30	2.448e-30	-29.564	-29.611	-0.047	(0)
Cl(1)	5.626e-39					
HClO	3.331e-39	3.331e-39	-38.477	-38.477	0.000	(0)
ClO-	2.295e-39	2.057e-39	-38.639	-38.687	-0.047	(0)
Cl(3)	0.000e+00					
ClO2-	0.000e+00	0.000e+00	-66.922	-66.970	-0.047	(0)
HClO2	0.000e+00	0.000e+00	-71.160	-71.160	0.000	(0)
Cl(5)	0.000e+00					
ClO3-	0.000e+00	0.000e+00	-81.353	-81.401	-0.048	(0)
Cl(7)	0.000e+00					
ClO4-	0.000e+00	0.000e+00	-100.085	-100.134	-0.048	(0)
ZnClO4+	0.000e+00	0.000e+00	-105.282	-105.329	-0.047	(0)
Cu(1)	4.189e-10					
Cu+	4.119e-10	3.693e-10	-9.385	-9.433	-0.047	(0)
CuCl2-	6.916e-12	6.201e-12	-11.160	-11.208	-0.047	(0)
CuCl3-2	3.113e-14	2.005e-14	-13.507	-13.698	-0.191	(0)
Cu(2)	3.775e-07					
CuCO3	3.525e-07	3.525e-07	-6.453	-6.453	0.000	(0)
Cu+2	1.021e-08	6.746e-09	-7.991	-8.171	-0.180	(0)
CuOH+	8.890e-09	7.970e-09	-8.051	-8.099	-0.047	(0)
Cu(CO3)2-2	5.341e-09	3.440e-09	-8.272	-8.463	-0.191	(0)
CuSO4	5.099e-10	5.099e-10	-9.293	-9.293	0.000	(0)
CuCl+	1.036e-11	9.290e-12	-10.985	-11.032	-0.047	(0)
CuCO3(OH)2-2	2.441e-12	1.572e-12	-11.612	-11.804	-0.191	(0)
CuF+	2.346e-12	2.103e-12	-11.630	-11.677	-0.047	(0)
CuCl2	2.463e-15	2.463e-15	-14.609	-14.609	0.000	(0)

CuO2-2	1.024e-18	6.595e-19	-17.990	-18.181	-0.191	(0)
CuCl4-2	1.819e-26	1.171e-26	-25.740	-25.931	-0.191	(0)
F	2.265e-05					
F-	2.198e-05	1.967e-05	-4.658	-4.706	-0.048	(0)
MgF+	5.170e-07	4.635e-07	-6.287	-6.334	-0.047	(0)
CaF+	1.200e-07	1.076e-07	-6.921	-6.968	-0.047	(0)
MnF+	2.929e-08	2.626e-08	-7.533	-7.581	-0.047	(0)
NaF	1.871e-09	1.871e-09	-8.728	-8.728	0.000	(0)
HF	1.318e-09	1.318e-09	-8.880	-8.880	0.000	(0)
AlF2+	1.573e-10	1.410e-10	-9.803	-9.851	-0.047	(0)
FeF+	1.232e-10	1.104e-10	-9.909	-9.957	-0.047	(0)
ZnF+	1.044e-10	9.364e-11	-9.981	-10.029	-0.047	(0)
AlF3	3.491e-11	3.491e-11	-10.457	-10.457	0.000	(0)
AlF+2	2.777e-11	1.801e-11	-10.556	-10.745	-0.188	(0)
CuF+	2.346e-12	2.103e-12	-11.630	-11.677	-0.047	(0)
BaF+	1.790e-12	1.605e-12	-11.747	-11.795	-0.047	(0)
AlF4-	1.924e-13	1.725e-13	-12.716	-12.763	-0.047	(0)
HF2-	7.004e-15	6.280e-15	-14.155	-14.202	-0.047	(0)
BF2(OH)2-	7.325e-16	6.567e-16	-15.135	-15.183	-0.047	(0)
FeF+2	1.069e-16	6.932e-17	-15.971	-16.159	-0.188	(0)
FeF2+	2.461e-17	2.206e-17	-16.609	-16.656	-0.047	(0)
H2F2	4.321e-18	4.321e-18	-17.364	-17.364	0.000	(0)
BF3OH-	2.683e-21	2.406e-21	-20.571	-20.619	-0.047	(0)
BF4-	1.527e-28	1.369e-28	-27.816	-27.864	-0.047	(0)
Fe(2)	1.236e-06					
FeHCO3+	7.734e-07	6.934e-07	-6.112	-6.159	-0.047	(0)
Fe+2	3.710e-07	2.451e-07	-6.431	-6.611	-0.180	(0)
FeCO3	7.624e-08	7.624e-08	-7.118	-7.118	0.000	(0)
FeSO4	1.282e-08	1.282e-08	-7.892	-7.892	0.000	(0)
FeOH+	1.980e-09	1.775e-09	-8.703	-8.751	-0.047	(0)
FeF+	1.232e-10	1.104e-10	-9.909	-9.957	-0.047	(0)
FeCl+	1.003e-10	8.989e-11	-9.999	-10.046	-0.047	(0)
Fe(OH)2	3.230e-13	3.230e-13	-12.491	-12.491	0.000	(0)
Fe(OH)3-	3.285e-16	2.945e-16	-15.483	-15.531	-0.047	(0)
FeCl2	2.428e-16	2.428e-16	-15.615	-15.615	0.000	(0)
FeCl4-2	2.761e-22	1.778e-22	-21.559	-21.750	-0.191	(0)
Fe(OH)4-2	1.047e-23	6.745e-24	-22.980	-23.171	-0.191	(0)
Fe(3)	3.136e-06					
Fe(OH)3	2.824e-06	2.824e-06	-5.549	-5.549	0.000	(0)
Fe(OH)2+	2.940e-07	2.636e-07	-6.532	-6.579	-0.047	(0)
Fe(OH)4-	1.812e-08	1.625e-08	-7.742	-7.789	-0.047	(0)
FeOH+2	5.360e-11	3.475e-11	-10.271	-10.459	-0.188	(0)
FeCO3+	8.293e-12	7.435e-12	-11.081	-11.129	-0.047	(0)
Fe+3	5.548e-16	2.350e-16	-15.256	-15.629	-0.373	(0)
FeF+2	1.069e-16	6.932e-17	-15.971	-16.159	-0.188	(0)
FeF2+	2.461e-17	2.206e-17	-16.609	-16.656	-0.047	(0)
FeSO4+	8.367e-18	7.502e-18	-17.077	-17.125	-0.047	(0)
FeNO3+2	1.169e-18	7.578e-19	-17.932	-18.120	-0.188	(0)
Fe2(OH)2+4	1.754e-19	3.251e-20	-18.756	-19.488	-0.732	(0)
Fe(SO4)2-	4.667e-20	4.184e-20	-19.331	-19.378	-0.047	(0)
FeCl+2	3.040e-20	1.971e-20	-19.517	-19.705	-0.188	(0)
FeCl2+	8.961e-21	8.034e-21	-20.048	-20.095	-0.047	(0)
Fe3(OH)4+5	2.400e-23	1.790e-24	-22.620	-23.747	-1.127	(0)
FeCl4-	2.730e-30	2.448e-30	-29.564	-29.611	-0.047	(0)
H(0)	3.016e-26					
H2	1.508e-26	1.512e-26	-25.822	-25.820	0.001	(0)
K	2.559e-05					
K+	2.552e-05	2.280e-05	-4.593	-4.642	-0.049	(0)
KSO4-	6.772e-08	6.072e-08	-7.169	-7.217	-0.047	(0)
KCl	3.855e-10	3.855e-10	-9.414	-9.414	0.000	(0)
KOH	1.811e-12	1.811e-12	-11.742	-11.742	0.000	(0)
KHSO4	2.339e-15	2.339e-15	-14.631	-14.631	0.000	(0)
Mg	1.605e-03					
Mg+2	1.445e-03	9.765e-04	-2.840	-3.010	-0.170	(0)
MgSO4	8.603e-05	8.603e-05	-4.065	-4.065	0.000	(0)
MgHCO3+	6.818e-05	6.113e-05	-4.166	-4.214	-0.047	(0)
MgCO3	5.659e-06	5.659e-06	-5.247	-5.247	0.000	(0)

MgF+	5.170e-07	4.635e-07	-6.287	-6.334	-0.047	(0)
MgCl+	4.281e-07	3.838e-07	-6.368	-6.416	-0.047	(0)
MgB(OH)4+	1.054e-08	9.446e-09	-7.977	-8.025	-0.047	(0)
Mg4(OH)4+4	2.400e-22	4.450e-23	-21.620	-22.352	-0.732	(0)
Mn(2)	9.106e-05					
Mn+2	7.509e-05	4.961e-05	-4.124	-4.304	-0.180	(0)
MnCO3	9.514e-06	9.514e-06	-5.022	-5.022	0.000	(0)
MnSO4	4.038e-06	4.038e-06	-5.394	-5.394	0.000	(0)
MnHCO3+	2.271e-06	2.036e-06	-5.644	-5.691	-0.047	(0)
MnCl+	5.932e-08	5.318e-08	-7.227	-7.274	-0.047	(0)
MnOH+	3.258e-08	2.921e-08	-7.487	-7.534	-0.047	(0)
MnF+	2.929e-08	2.626e-08	-7.533	-7.581	-0.047	(0)
MnNO3+	2.828e-08	2.535e-08	-7.549	-7.596	-0.047	(0)
Mn2(OH)3+	4.153e-11	3.723e-11	-10.382	-10.429	-0.047	(0)
Mn(NO3)2	2.054e-11	2.054e-11	-10.687	-10.687	0.000	(0)
Mn2OH+3	4.062e-12	1.553e-12	-11.391	-11.809	-0.418	(0)
Mn(OH)2	1.642e-12	1.642e-12	-11.785	-11.785	0.000	(0)
MnCl3-	3.284e-15	2.944e-15	-14.484	-14.531	-0.047	(0)
Mn(OH)3-	3.935e-17	3.528e-17	-16.405	-16.452	-0.047	(0)
Mn(OH)4-2	1.062e-23	6.843e-24	-22.974	-23.165	-0.191	(0)
Mn(3)	3.462e-26					
Mn+3	3.462e-26	1.323e-26	-25.461	-25.878	-0.418	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-47.681	-47.872	-0.191	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-53.180	-53.228	-0.048	(0)
N(5)	3.629e-04					
NO3-	3.609e-04	3.224e-04	-3.443	-3.492	-0.049	(0)
CaNO3+	1.939e-06	1.739e-06	-5.712	-5.760	-0.047	(0)
MnNO3+	2.828e-08	2.535e-08	-7.549	-7.596	-0.047	(0)
BaNO3+	3.383e-10	3.033e-10	-9.471	-9.518	-0.047	(0)
Mn(NO3)2	2.054e-11	2.054e-11	-10.687	-10.687	0.000	(0)
HNO3	7.362e-13	7.362e-13	-12.133	-12.133	0.000	(0)
FeNO3+2	1.169e-18	7.578e-19	-17.932	-18.120	-0.188	(0)
Na	1.001e-03					
Na+	9.919e-04	8.893e-04	-3.004	-3.051	-0.047	(0)
NaHCO3	6.856e-06	6.856e-06	-5.164	-5.164	0.000	(0)
NaSO4-	2.162e-06	1.938e-06	-5.665	-5.713	-0.047	(0)
NaCl	7.868e-08	7.868e-08	-7.104	-7.104	0.000	(0)
NaCO3-	1.901e-08	1.704e-08	-7.721	-7.768	-0.047	(0)
NaF	1.871e-09	1.871e-09	-8.728	-8.728	0.000	(0)
NaB(OH)4	2.029e-10	2.029e-10	-9.693	-9.693	0.000	(0)
NaAlO2	5.545e-11	5.545e-11	-10.256	-10.256	0.000	(0)
NaOH	3.386e-11	3.386e-11	-10.470	-10.470	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-40.556	-40.555	0.001	(0)
S(6)	6.564e-04					
SO4-2	5.122e-04	3.299e-04	-3.291	-3.482	-0.191	(0)
MgSO4	8.603e-05	8.603e-05	-4.065	-4.065	0.000	(0)
CaSO4	5.184e-05	5.184e-05	-4.285	-4.285	0.000	(0)
MnSO4	4.038e-06	4.038e-06	-5.394	-5.394	0.000	(0)
NaSO4-	2.162e-06	1.938e-06	-5.665	-5.713	-0.047	(0)
KSO4-	6.772e-08	6.072e-08	-7.169	-7.217	-0.047	(0)
ZnSO4	2.337e-08	2.337e-08	-7.631	-7.631	0.000	(0)
FeSO4	1.282e-08	1.282e-08	-7.892	-7.892	0.000	(0)
HSO4-	1.623e-09	1.455e-09	-8.790	-8.837	-0.047	(0)
CuSO4	5.099e-10	5.099e-10	-9.293	-9.293	0.000	(0)
AlSO4+	3.447e-14	3.091e-14	-13.463	-13.510	-0.047	(0)
KHSO4	2.339e-15	2.339e-15	-14.631	-14.631	0.000	(0)
Al(SO4)2-	8.828e-16	7.914e-16	-15.054	-15.102	-0.047	(0)
FeSO4+	8.367e-18	7.502e-18	-17.077	-17.125	-0.047	(0)
H2SO4	5.991e-20	5.991e-20	-19.223	-19.223	0.000	(0)
Fe(SO4)2-	4.667e-20	4.184e-20	-19.331	-19.378	-0.047	(0)
Zn	6.120e-07					
Zn+2	5.101e-07	3.371e-07	-6.292	-6.472	-0.180	(0)
ZnHCO3+	5.223e-08	4.683e-08	-7.282	-7.329	-0.047	(0)
ZnSO4	2.337e-08	2.337e-08	-7.631	-7.631	0.000	(0)

ZnCO3	1.551e-08	1.551e-08	-7.810	-7.810	0.000 (0)
ZnOH+	9.443e-09	8.466e-09	-8.025	-8.072	-0.047 (0)
Zn(OH)2	8.305e-10	8.305e-10	-9.081	-9.081	0.000 (0)
ZnCl+	3.180e-10	2.851e-10	-9.498	-9.545	-0.047 (0)
Zn(OH)Cl	1.116e-10	1.116e-10	-9.952	-9.952	0.000 (0)
ZnF+	1.044e-10	9.364e-11	-9.981	-10.029	-0.047 (0)
ZnCl2	1.676e-13	1.676e-13	-12.776	-12.776	0.000 (0)
Zn(OH)3-	6.576e-14	5.896e-14	-13.182	-13.229	-0.047 (0)
ZnCl3-	5.198e-17	4.661e-17	-16.284	-16.332	-0.047 (0)
Zn(OH)4-2	3.575e-19	2.302e-19	-18.447	-18.638	-0.191 (0)
ZnCl4-2	2.761e-19	1.778e-19	-18.559	-18.750	-0.191 (0)
ZnClO4+	0.000e+00	0.000e+00	-105.282	-105.329	-0.047 (0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al	-110.46	39.46	149.91	Al
Al(g)	-161.16	39.46	200.62	Al
Al2(SO4)3	-55.42	-36.52	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-38.08	-36.52	1.56	Al2(SO4)3:6H2O
AlF3	-9.89	-27.16	-17.27	AlF3
Alstonite	-2.30	0.29	2.58	BaCa(CO3)2
Alum-K	-19.67	-24.64	-4.97	KAl(SO4)2:12H2O
Alunite	-6.09	-6.56	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-2.10	-6.45	-4.35	CaSO4
Antarcticite	-13.66	-9.56	4.09	CaCl2:6H2O
Antlerite	-7.28	1.45	8.73	Cu3(SO4)(OH)4
Aphthitalite	-20.05	-23.94	-3.89	NaK3(SO4)2
Aragonite	0.15	2.12	1.97	CaCO3
Arcanite	-10.92	-12.77	-1.84	K2SO4
Artinite	-5.84	13.79	19.63	Mg2CO3(OH)2:3H2O
Atacamite	-9.38	4.88	14.26	Cu4Cl2(OH)6
Azurite	-8.73	0.39	9.12	Cu3(CO3)2(OH)2
B	-84.17	25.39	109.56	B
B(g)	-175.45	25.39	200.84	B
B2O3	-15.60	-10.06	5.55	B2O3
Ba	-113.16	28.07	141.23	Ba
Ba(OH)2:8H2O	-16.70	7.79	24.49	Ba(OH)2:8H2O
BaCl2	-15.75	-13.52	2.23	BaCl2
BaCl2:2H2O	-13.73	-13.52	0.21	BaCl2:2H2O
BaCl2:H2O	-14.35	-13.52	0.82	BaCl2:H2O
BaMnO4	-44.71	-54.80	-10.09	BaMnO4
BaO	-40.00	7.79	47.80	BaO
Barite	-0.40	-10.41	-10.01	BaSO4
Barytocalcite	-2.45	0.29	2.74	BaCa(CO3)2
Bassanite	-2.74	-6.45	-3.71	CaSO4:0.5H2O
BF3(g)	-38.25	-41.23	-2.98	BF3
Birnessite	-50.15	-135.70	-85.55	Mn8O14:5H2O
Bischofite	-14.00	-9.61	4.39	MgCl2:6H2O
Bixbyite	-6.63	-7.60	-0.96	Mn2O3
Bloedite	-13.60	-16.08	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	1.49	9.04	7.55	AlO2H
Borax	-23.53	-11.49	12.04	Na2(B4O5(OH)4):8H2O
Boric_acid	-4.87	-5.03	-0.16	B(OH)3
Brochantite	-7.43	7.99	15.42	Cu4(SO4)(OH)6
Brucite	-4.57	11.71	16.28	Mg(OH)2
Burkeite	-29.66	-20.18	9.49	Na6CO3(SO4)2
C	-33.22	30.93	64.15	C
C(g)	-150.84	30.93	181.77	C
Ca	-107.80	32.03	139.83	Ca
Ca(g)	-133.04	32.03	165.07	Ca
Ca2Al2O5:8H2O	-17.98	41.59	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-24.10	2.19	26.29	Ca2Cl2(OH)2:H2O
Ca3Al2O6	-59.69	53.34	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-62.49	77.99	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-42.17	65.09	107.25	Ca4Al2O7:13H2O

Ca4Al2O7:19H2O	-38.59	65.09	103.68 Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-42.64	25.69	68.33 Ca4Cl2(OH)6:13H2O
CaAl2O4	-17.07	29.83	46.91 CaAl2O4
CaAl2O4:10H2O	-8.16	29.83	37.99 CaAl2O4:10H2O
CaAl4O7	-20.67	47.92	68.59 CaAl4O7
Calcite	0.30	2.12	1.82 CaCO3
Carnallite	-21.82	-17.55	4.27 KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.91	-6.45	-3.54 CaSO4:0.5H2O
Chalcanthite	-9.02	-11.65	-2.63 CuSO4:5H2O
Chalcocyanite	-14.56	-11.65	2.91 CuSO4
Chloromagnesite	-31.42	-9.61	21.82 MgCl2
Cl2(g)	-44.59	-41.59	2.99 Cl2
CO2(g)	-1.80	-9.63	-7.83 CO2
Colemanite	-28.18	-6.66	21.51 Ca2B6O11:5H2O
Corundum	-0.21	18.08	18.29 Al2O3
Cu	-4.67	26.83	31.50 Cu
Cu(g)	-56.83	26.83	83.66 Cu
CuCl2	-18.49	-14.77	3.72 CuCl2
CuF	-21.22	-14.14	7.08 CuF
CuF2	-16.96	-17.58	-0.62 CuF2
CuF2:2H2O	-13.03	-17.58	-4.55 CuF2:2H2O
Cuprite	-2.24	-4.15	-1.91 Cu2O
Dawsonite	-0.62	3.72	4.34 NaAlCO3(OH)2
Delafossite	10.81	4.38	-6.44 CuFeO2
Diaspore	1.90	9.04	7.15 AlHO2
Dolomite	1.73	4.20	2.47 CaMg(CO3)2
Dolomite-dis	0.19	4.20	4.01 CaMg(CO3)2
Dolomite-ord	1.74	4.20	2.46 CaMg(CO3)2
Epsomite	-4.53	-6.49	-1.96 MgSO4:7H2O
Ettringite	-28.48	33.99	62.46 Ca6Al2(SO4)3(OH)12:26H2O
F2(g)	-100.12	-44.41	55.71 F2
Fe	-30.63	28.39	59.02 Fe
Fe(OH)2	-5.79	8.11	13.89 Fe(OH)2
Fe(OH)3	0.81	6.45	5.64 Fe(OH)3
Fe2(SO4)3	-44.75	-41.70	3.05 Fe2(SO4)3
FeF2	-13.60	-16.02	-2.42 FeF2
FeF3	-10.49	-29.75	-19.26 FeF3
FeO	-5.41	8.11	13.52 FeO
Ferrite-Ca	3.16	24.65	21.50 CaFe2O4
Ferrite-Cu	9.17	19.45	10.28 CuFe2O4
Ferrite-Dicalcium	-20.39	36.41	56.80 Ca2Fe2O5
Ferrite-Mg	3.59	24.61	21.02 MgFe2O4
Ferrite-Zn	9.45	21.15	11.70 ZnFe2O4
FeSO4	-12.70	-10.09	2.61 FeSO4
Fluorite	-2.31	-12.38	-10.07 CaF2
Frankdicksonite	-10.58	-16.34	-5.76 BaF2
Gaylussite	-10.05	1.11	11.16 CaNa2(CO3)2:5H2O
Gibbsite	1.30	9.04	7.74 Al(OH)3
Glauberite	-10.56	-16.03	-5.47 Na2Ca(SO4)2
Goethite	5.92	6.45	0.53 FeOOH
Gypsum	-1.92	-6.45	-4.53 CaSO4:2H2O
H2(g)	-22.72	-25.82	-3.10 H2
H2O(g)	-1.59	-0.00	1.59 H2O
Halite	-7.91	-6.35	1.56 NaCl
Hausmannite	-7.33	2.82	10.14 Mn3O4
HCl(g)	-16.96	-10.66	6.30 HCl
Hematite	12.83	12.90	0.08 Fe2O3
Hercynite	-2.61	26.19	28.80 FeAl2O4
Hexahydrite	-4.77	-6.49	-1.73 MgSO4:6H2O
Huntite	-1.85	8.37	10.22 CaMg3(CO3)4
Hydroboracite	-27.07	-6.70	20.36 MgCaB6O11:6H2O
Hydromagnesite	-10.71	20.03	30.74 Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-21.31	-9.56	11.75 CaCl2
Hydrozincite	-8.33	21.98	30.31 Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14 H2O
Jarosite	-4.92	-14.33	-9.41 KFe3(SO4)2(OH)6
Jarosite-Na	-7.29	-12.74	-5.45 NaFe3(SO4)2(OH)6

K -58.12 12.86 70.98 K
K(g) -68.72 12.86 81.58 K
K2CO3:1.5H2O -17.57 -4.19 13.38 K2CO3:1.5H2O
K2O -78.60 5.44 84.04 K2O
K3H(SO4)2 -24.63 -28.25 -3.62 K3H(SO4)2
K8H4(CO3)6:3H2O -63.74 -36.03 27.71 K8H4(CO3)6:3H2O
Kainite -14.12 -14.43 -0.31 KMgClSO4:3H2O
KAl(SO4)2 -27.92 -24.64 3.27 KAl(SO4)2
Kalicinite -7.19 -6.91 0.28 KHCO3
Katoite -25.61 53.34 78.94 Ca3Al2H12O12
Kieserite -6.23 -6.49 -0.27 MgSO4:H2O
KMgCl3 -38.79 -17.55 21.25 KMgCl3
KMgCl3:2H2O -31.51 -17.55 13.96 KMgCl3:2H2O
KNaCO3:6H2O -12.86 -2.60 10.26 KNaCO3:6H2O
Lansfordite -2.76 2.08 4.84 MgCO3:5H2O
Lawrencite -22.26 -13.21 9.05 FeCl2
Leonite -15.15 -19.26 -4.11 K2Mg(SO4)2:4H2O
Lime -20.82 11.75 32.57 CaO
Magnesite -0.19 2.08 2.27 MgCO3
Magnetite 10.59 21.01 10.42 Fe3O4
Malachite -2.43 3.47 5.90 Cu2CO3(OH)2
Manganite -3.63 -3.80 -0.16 MnO(OH)
Manganosite -7.50 10.42 17.92 MnO
Mayenite -226.55 267.60 494.15 Ca12Al14O33
Melanterite -7.69 -10.09 -2.40 FeSO4:7H2O
Mercallite -14.04 -15.48 -1.44 KHSO4
Mg -90.53 31.99 122.52 Mg
Mg(g) -110.26 31.99 142.25 Mg
Mg1.25SO4(OH)0.5:0.5H2O -8.76 -3.56 5.20 Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH) -9.85 -0.64 9.21 Mg1.5SO4(OH)
MgCl2:2H2O -22.34 -9.61 12.73 MgCl2:2H2O
MgCl2:4H2O -16.91 -9.61 7.30 MgCl2:4H2O
MgCl2:H2O -25.68 -9.61 16.07 MgCl2:H2O
MgOHCl -14.84 1.05 15.89 MgOHCl
MgSO4 -11.32 -6.49 4.83 MgSO4
Mirabilite -8.43 -9.58 -1.15 Na2SO4:10H2O
Misenite -94.59 -105.67 -11.08 K8H6(SO4)7
Mn -52.24 30.69 82.93 Mn
Mn(OH)2(am) -4.89 10.42 15.31 Mn(OH)2
Mn(OH)3 -10.14 -3.80 6.34 Mn(OH)3
MnCl2:2H2O -14.90 -10.90 4.00 MnCl2:2H2O
MnCl2:4H2O -13.65 -10.90 2.75 MnCl2:4H2O
MnCl2:H2O -16.44 -10.90 5.54 MnCl2:H2O
MnO2(gamma) -9.96 -26.09 -16.13 MnO2
MnSO4 -10.39 -7.79 2.61 MnSO4
Molysite -38.99 -25.52 13.47 FeCl3
Monohydrocalcite -0.55 2.12 2.68 CaCO3:H2O
Na -52.92 14.45 67.37 Na
Na(g) -66.41 14.45 80.86 Na
Na2CO3 -12.17 -1.01 11.16 Na2CO3
Na2CO3:7H2O -10.95 -1.01 9.94 Na2CO3:7H2O
Na2O -58.80 8.62 67.42 Na2O
Na3H(SO4)2 -22.59 -23.48 -0.89 Na3H(SO4)2
Na4Ca(SO4)3:2H2O -19.72 -25.62 -5.89 Na4Ca(SO4)3:2H2O
NaFeO2 -9.12 10.76 19.88 NaFeO2
Nahcolite -5.18 -5.32 -0.14 NaHCO3
Nantokite -5.96 -12.73 -6.77 CuCl
Natron -10.60 -1.01 9.59 Na2CO3:10H2O
Nesquehonite -3.21 2.08 5.29 MgCO3:3H2O
Niter -7.91 -8.13 -0.22 KNO3
Nitrobarite -11.42 -13.91 -2.49 Ba(NO3)2
NO2(g) -9.06 -0.71 8.35 NO2
O2(g) -37.66 -40.56 -2.89 O2
Oxychloride-Mg -13.07 12.76 25.83 Mg2Cl(OH)3:4H2O
Pentahydrite -5.11 -6.49 -1.39 MgSO4:5H2O
Periclase -9.62 11.71 21.33 MgO
Picromerite -14.82 -19.26 -4.44 K2Mg(SO4)2:6H2O

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  Pirssonite      -10.21      1.11   11.32  Na2Ca(CO3)2:2H2O
  Polyhalite      -17.85    -32.16  -14.31  K2MgCa2(SO4)4:2H2O
  Portlandite     -10.80     11.75   22.55  Ca(OH)2
  Pyrolusite       -8.43    -26.09  -17.66  MnO2
  Rhodochrosite     1.01      0.79   -0.22  MnCO3
  Scacchite       -19.64    -10.90    8.74  MnCl2
  Sellaite         -2.98    -12.42   -9.44  MgF2
  Siderite         -1.30     -1.52   -0.22  FeCO3
  Smithsonite      -1.82     -1.38    0.44  ZnCO3
  Spinel           -7.81     29.79   37.61  Al2MgO4
  Starkeyite       -5.49     -6.49   -1.00  MgSO4:4H2O
  Sylvite          -8.77     -7.94    0.83  KCl
  Syngenite       -11.62    -19.22   -7.60  K2Ca(SO4)2:H2O
  Tachyhydrite    -45.92    -28.78   17.14  Mg2CaCl6:12H2O
  Tenorite         -1.10      6.55    7.65  CuO
  Thenardite       -9.23     -9.58   -0.36  Na2SO4
  Thermonatrite   -11.95     -1.01   10.94  Na2CO3:H2O
  Todorokite      -39.56    -85.38  -45.82  Mn7O12:3H2O
  Trona-K         -21.10     -9.51   11.59  K2NaH(CO3)2:2H2O
  Witherite         1.18     -1.83   -3.02  BaCO3
  Wustite          -4.90      7.50   12.40  Fe.947O
  Zincite          -2.95      8.25   11.20  ZnO
  Zn              -40.26     28.53   68.79  Zn
  Zn(BO2)2        -10.12     -1.81    8.31  Zn(BO2)2
  Zn(ClO4)2:6H2O -212.37   -206.74    5.63  Zn(ClO4)2:6H2O
  Zn(g)           -56.88     28.53   85.41  Zn
  Zn(NO3)2:6H2O   -16.86    -13.46    3.40  Zn(NO3)2:6H2O
  Zn(OH)2(beta)    -3.68      8.25   11.93  Zn(OH)2
  Zn(OH)2(epsilon) -3.41      8.25   11.66  Zn(OH)2
  Zn(OH)2(gamma)   -3.64      8.25   11.88  Zn(OH)2
  Zn2(OH)3Cl       -9.46      5.84   15.29  Zn2(OH)3Cl
  Zn2SO4(OH)2      -9.29     -1.71    7.58  Zn2SO4(OH)2
  Zn3O(SO4)2       -30.75    -11.66   19.09  Zn3O(SO4)2
  Zn5(NO3)2(OH)8   -23.13     19.53   42.67  Zn5(NO3)2(OH)8
  ZnCl2            -20.15    -13.07    7.08  ZnCl2
  ZnCO3:H2O         -1.52     -1.38    0.14  ZnCO3:H2O
  ZnF2             -15.39    -15.88   -0.49  ZnF2
  ZnSO4            -13.49     -9.95    3.53  ZnSO4
  ZnSO4:6H2O        -8.25     -9.95   -1.70  ZnSO4:6H2O
  ZnSO4:7H2O        -8.08     -9.95   -1.88  ZnSO4:7H2O
  ZnSO4:H2O         -9.40     -9.95   -0.55  ZnSO4:H2O

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 5.
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End of Run after 0.416 Seconds.
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(last page)