What is Comet?

Rocks are mixtures of minerals, and minerals are stoichiometric combinations of elements. Comet (COgnitive Mineralogical Evaluation Tool) is a mass balance calculation system that estimates weight percent of minerals, from an assay table containing measured weight percent of elements. From your laboratory analyses of drill core or RC drill chips, Comet will calculate percentages of quartz, mica, chlorite, feldspars, pyrite etc, back-calculate whole rock SiO2 even where silica was not analysed, and a range of petrophysical parameters.

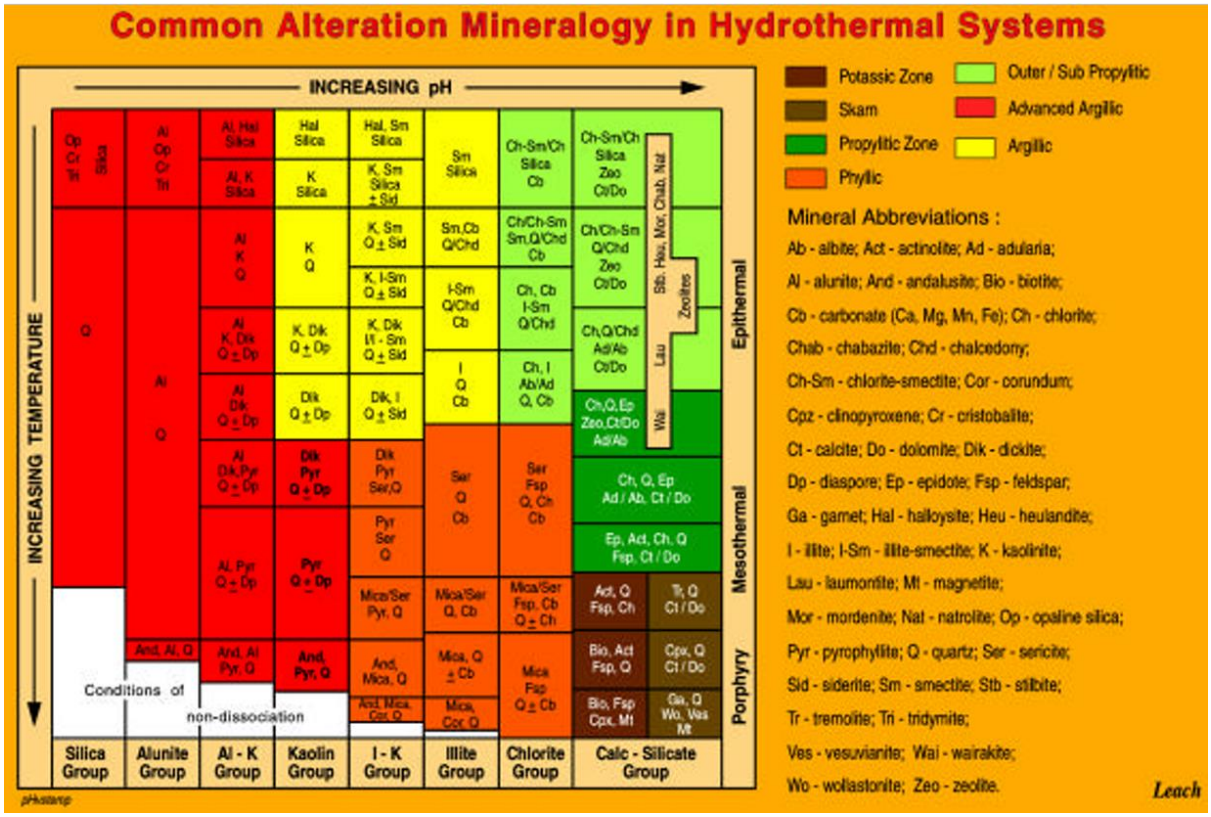
Consistent and accurate logging of drill core and chips is critical to building fit for purpose resource models and quantifying variability of orebodies. Visual logging by geologists is too inconsistent to allow the creation of accurate models. This has led to a proliferation of automated core logging systems. These core logging systems add significantly to the total cost and are often slow and subjective. Comet is designed to utilize the vast amount of 4 acid digest ICP assay data collected by exploration and mining companies to create a quantitative, fast, and consistent alternative.

Understanding the 3D distribution of minerals is important in exploration, resource estimation, engineering, mineral processing and environmental management.

How does it work?

Comet is a mass balance calculation. It starts with a table of minerals that are present in the system and the compositions of those minerals. It finds a solution where the sum of the components of the minerals is equal to the measured abundances of the elements. Mathematically, there are more variables than constraints, so there are an infinite number of solutions where this condition is met.

Think of an analogy in metamorphic petrology; facies vary from lower to middle to upper greenschist to amphibolite grade. The same rock composition can generate vastly different mineral assemblages. In hydrothermal environments, low temperature systems form clay minerals, mid-temperature systems form mostly white mica and chlorite, high temperature systems form black micas and feldspars. The famous diagram by Terry Leach and Greg Corbett illustrates the differences in mineralogy as a function of temperature.



Comet works on an optimization routine. It uses the thermodynamic properties of minerals to find the solution where the sum of the Gibbs Free Energy per unit mass of minerals is a minimum value. Think of the Gibbs Free Energy as a probability factor for the formation of one mineral relative to another.

Trying to predict modal mineralogy from assays in nothing new. The CIPW norm method was developed in 1902. It was created by Whitman Cross, Joseph P. Iddings, Louis V. Pirsson, and Henry S. Washington, who are often referred to as the "CIPW" authors. The method provides a way to calculate a standard mineral composition for igneous rocks based on their chemical analysis. Think of Comet as a sophisticated CIPW analogue for hydrothermally altered rocks that accounts for different hydrothermal environments and solid solution variability of key minerals.

There have been numerous attempts before now to create systems like Comet, but they all had limitations. In addition to the non-uniqueness of solutions, the other problem is that most common hydrothermal minerals (white mica, chlorite, biotite, alkali feldspar) are minerals that do not have fixed compositions, and the compositions will vary throughout a hydrothermal system. The generic formulae of these minerals are written as;

Muscovite $KAl_3Si_3O_{10}(OH)_2$

Chlorite $(Fe,Mg)_5Al_2Si_3O_{10}(OH)_8$

Biotite $K(Fe,Mg)_3AlSi_3O_{10}(OH)_2$

Measured mineral chemistry from hydrothermal systems shows that these minerals rarely have compositions like these idealized formulae. Comet tries to model chlorite and biotite by using the sum of likely end-member compositions. We also have a method to estimate white mica compositions based on a ratio of cations from the whole rock analysis. That means different mineral compositions are used for each row of data.

The thermodynamic constraints within Comet are based on an internally consistent compilation from Holland and Powell, (1998). Testing Comet on drill hole data bases from more than 100 mineral deposits around the world has highlighted that there are a few minerals for which the Holland and Powell parameters do not produce plausible outcomes. Consequently, some deltaG values from Holland and Powell have been modified to generate more realistic results.

One of the inputs that is required to run Comet is an estimate of the temperature of the system at the main ore-forming stage. As a rule of thumb, use the Corbett and Leach diagram as a guide. Look at the mineral assemblages described in this diagram and decide on a realistic temperature window.

Porphyry	350°
Mesothermal	300°
Epithermal	250°
Outflow from Epithermal	200°

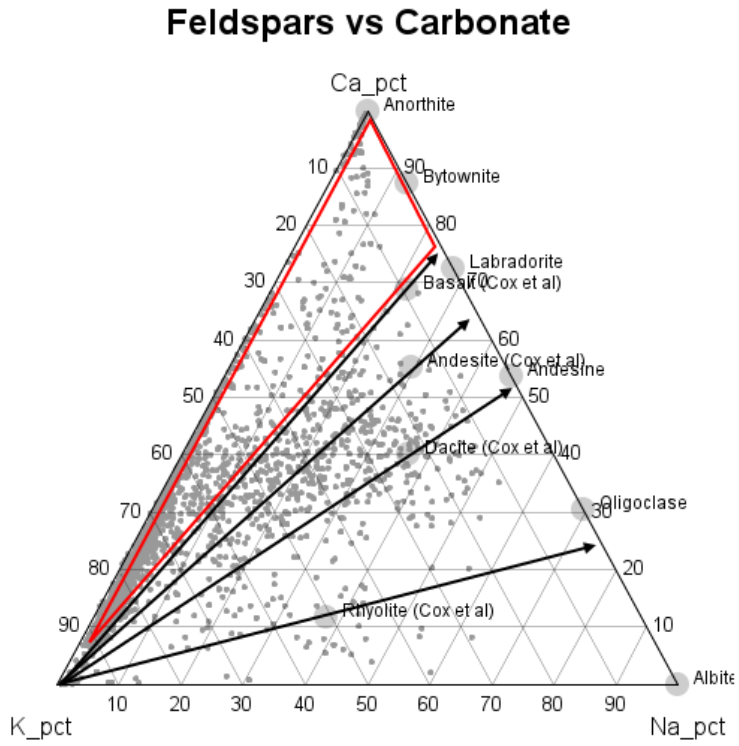
What kind of data do I need?

The input required for Comet is whole rock geochemical analyses. The type of suitable data most commonly collected by companies is 4 acid digest ICP. This analytical method does not include SiO2, but that does not make a big difference to the calculated results. Whole rock laboratory XRF is also very acceptable (even better than ICP). pXRF is not suitable because the error bars are too great.

The minimum suite of elements required is Al, Ca, Fe, K, Mg, Na, S. It is preferable to also include Ba, Cu, Mn, P, Pb, Zn, and other elements that have an abundance of >0.1% somewhere within the database. The required input format is a csv file that includes Sample_ID and all the elements in units of percent. There should be no blank cells, no negative values, no symbols (eg <), no values >100, and the sum of the elements in every row must be <100.

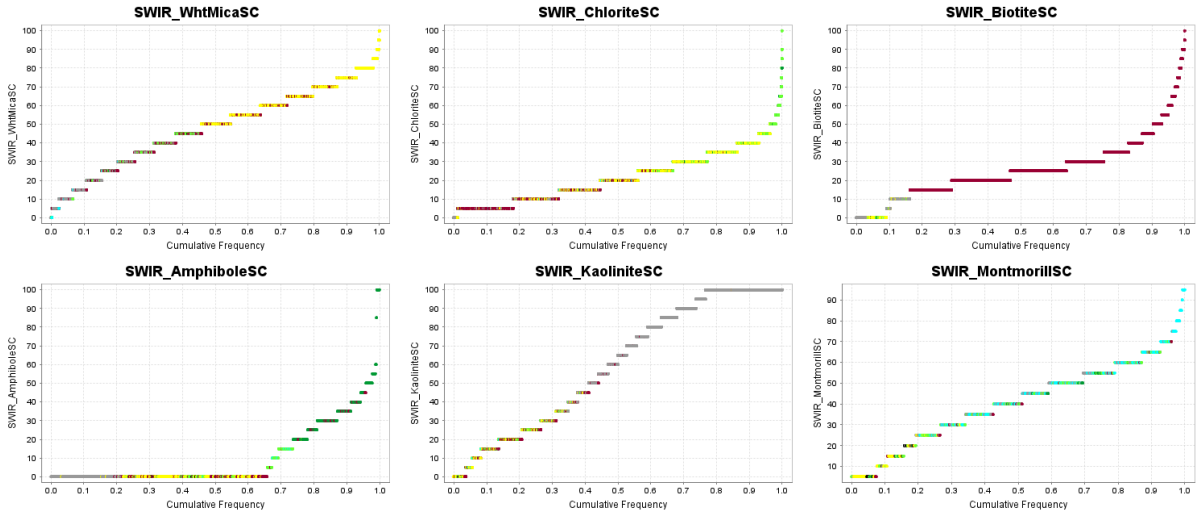
How do I know what minerals to include in the calculation?

For every system, include quartz, feldspar, white mica, chlorite, pyrite, magnetite (Fe-oxide) and kaolinite. Feldspar is modelled as orthoclase, albite, plagioclase, and Ba is also calculated as a component of feldspar, unless barite is present in the system. Chlorite will include Fe and Mg endmembers, and Mn is calculated as a component of chlorite, unless Mn carbonates are present in the system. Ti is routinely included as one of the elements that is uploaded, and assigned to rutile. P is uploaded and assigned to apatite. Cu, Pb and Zn are calculated as chalcopyrite, galena and sphalerite unless you know there are other base metal minerals in the system with an abundance significant enough to warrant calculating them.



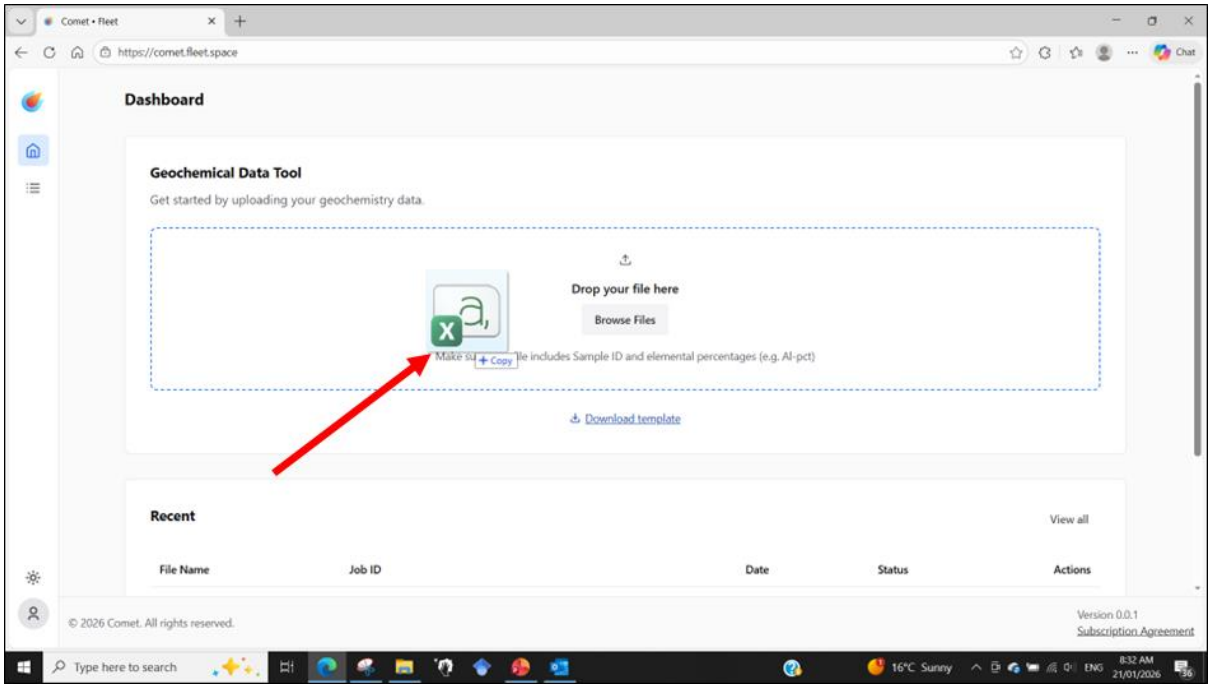
One of the screens in the Comet upload will ask what the most mafic rocks in your system are. This sets an upper limit to the amount of Ca that will be assigned to plagioclase. The effect of this can be seen in a Ca-K-Na ternary plot. If there are rocks with a Ca/Na ratio beyond the plagioclase composition appropriate for that rock type, it implies that those rocks must have carbonate or anhydrite.

You should be able to tell from visual logging whether the core contains biotite or amphibole. If SWIR data (aiSIRIS) or automated SWIR data is available, then it is recommended that you should look at this data in ioGAS. Create cumulative frequency plots of mineral_sc values or mineral_pxa values to get a quick overview of the minerals that are identified from spectral logging.

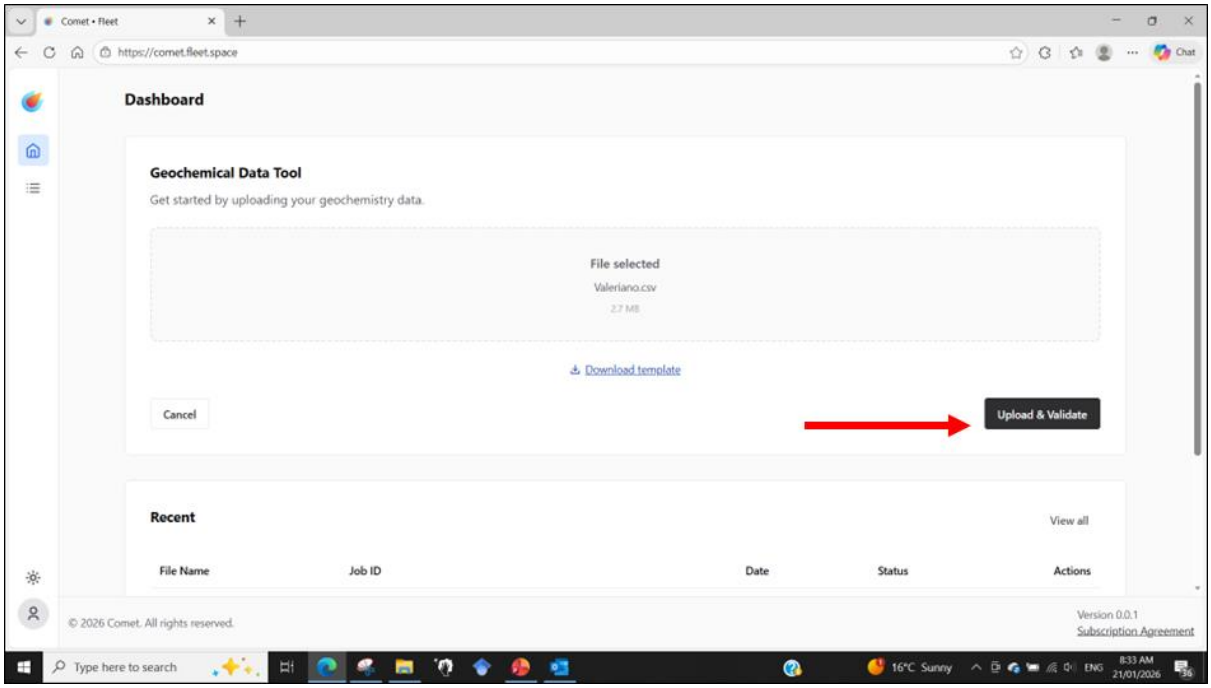


Using the software

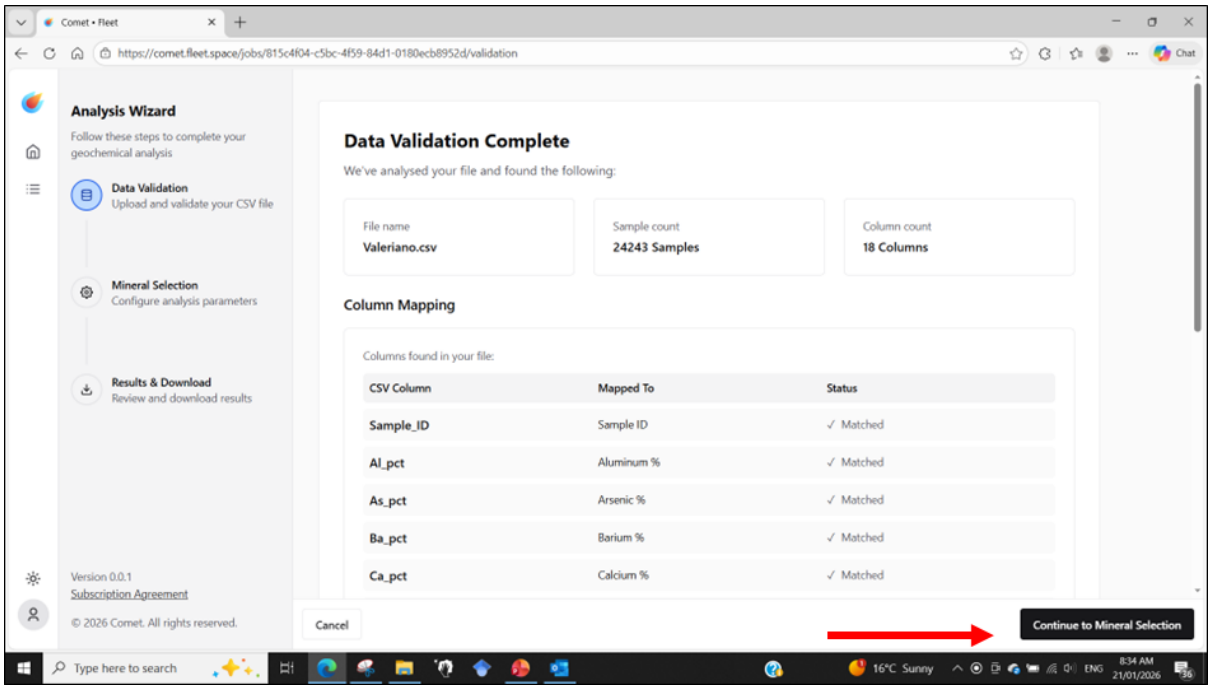
Log in to Comet.



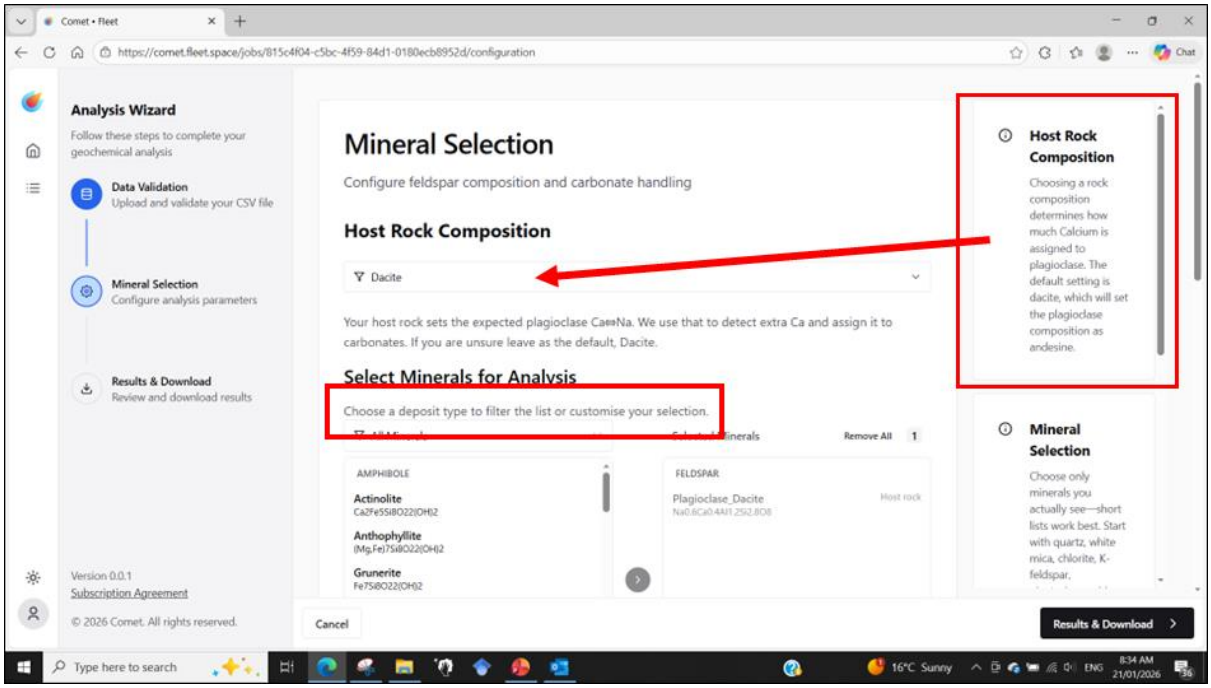
Drag and drop your csv file.



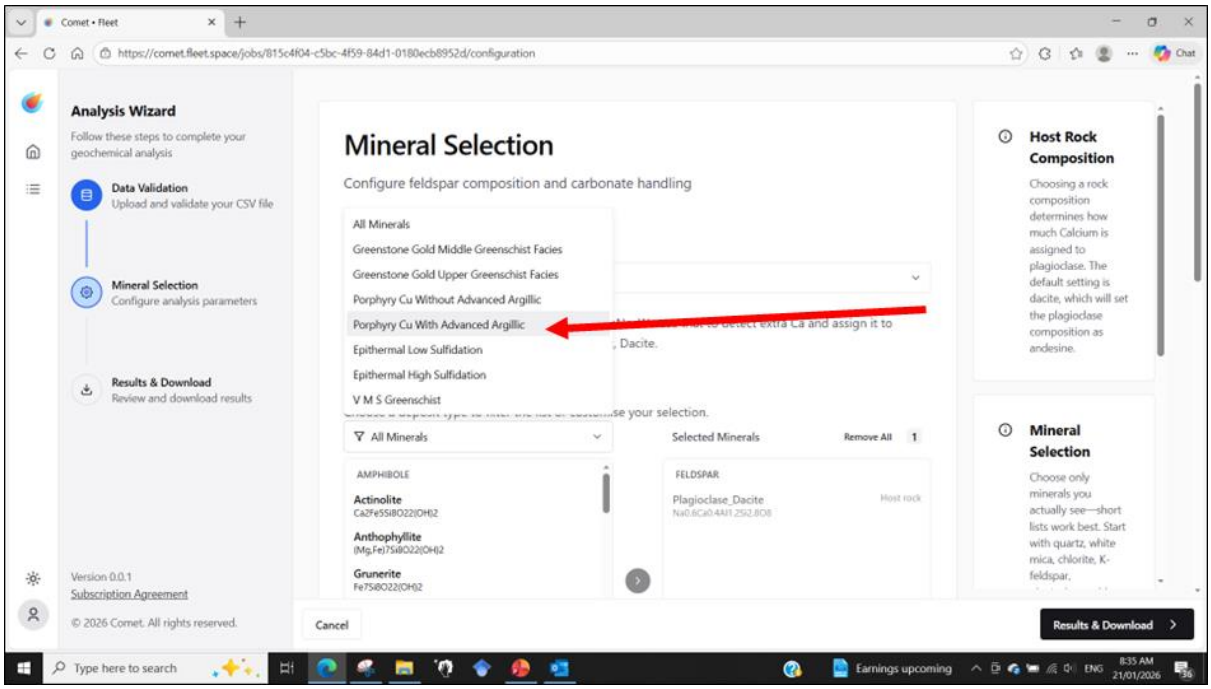
Upload and validate.



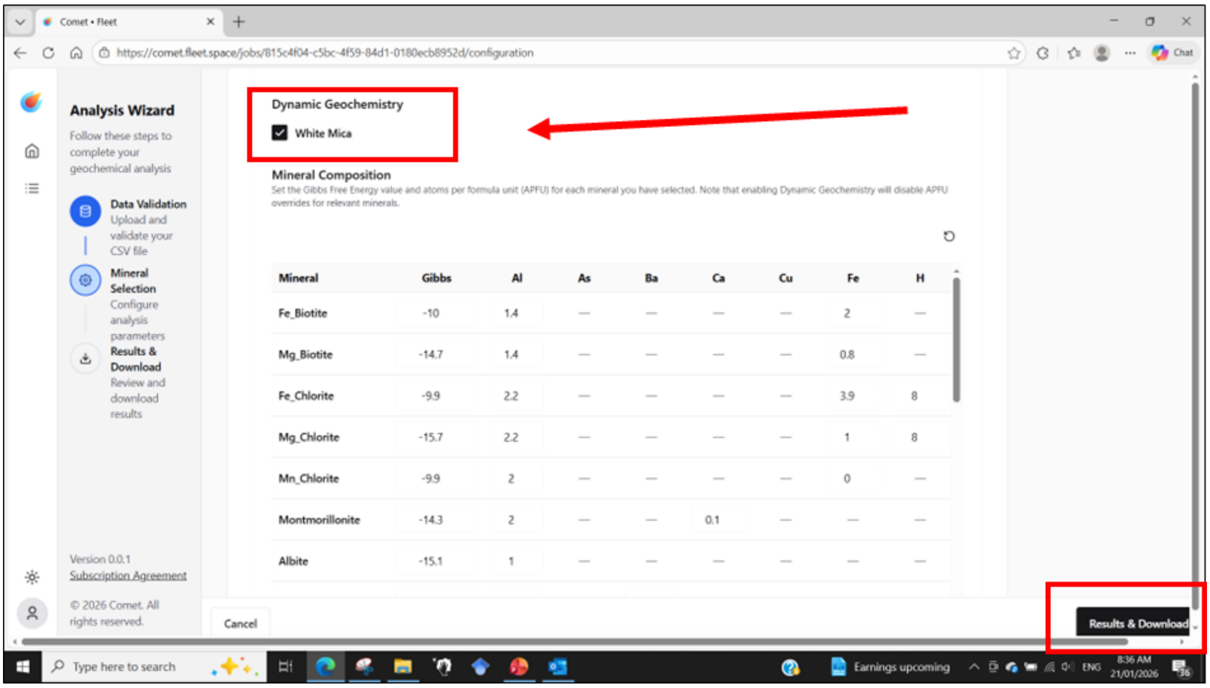
The software reads in the elements. It will report errors for incorrectly formatted data.



The next screen asks for the rock composition to set the maximum Ca content of plagioclase. The default is dacite with a plagioclase composition of $Na_{0.4}Ca_{0.6}Al_{1.6}Si_{2.4}O_8$



Comet includes some pre-selected mineral lists for a variety of mineral deposit types. This is included as a shortcut to building the initial mineral list and should be a prompt so that key minerals are not overlooked. Additional minerals can be added or removed from the selected list using the selection arrows.



Leave the white mica dynamic composition turned on. On this screen it is possible to manually override the Gibbs Free Energy “probability” factors. The atoms per formula unit numbers defining the mineral compositions can also be manually edited. At the bottom of the screen there is a slide bar to manually change the selected temperature for the hydrothermal system.

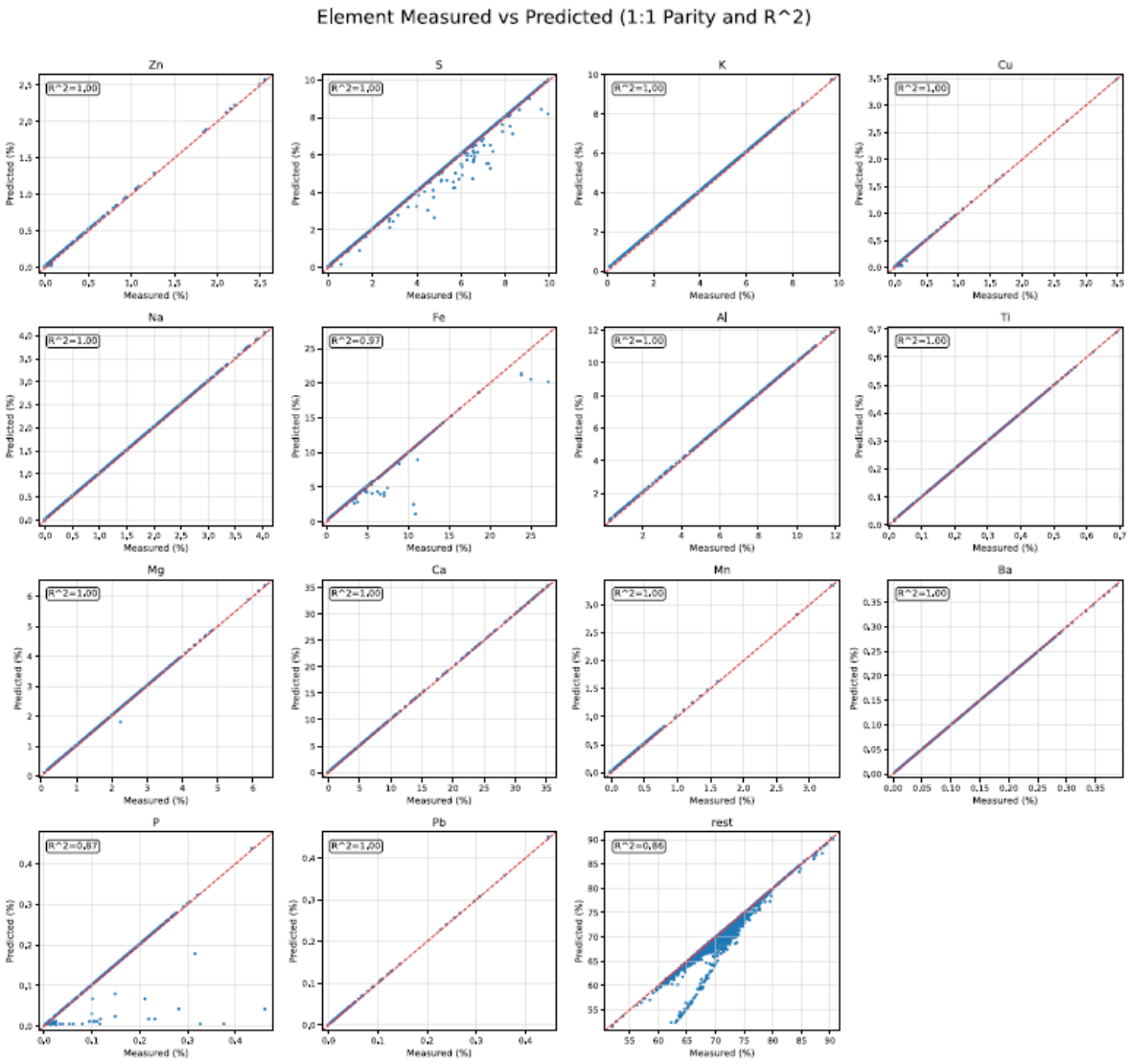
BU1 calculated_SiO2_pct

	F	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	BU	BV	BW	BX	BY	BZ	CA	CB
1	Sample_ID	Al_pct	Ba_pct	Ca_pct	Cu_pct	Fe_pct	K_pct	Mg_pct	Mn_pct	Na_pct	P_pct	Pb_pct	S_pct	Ti_pct	Zn_pct	calculated	Quartz_pct	Albite_pct	Ba_Feldsp	K_Feldspar	Plagioclase	Total Felds	Muscovite_
2	MP19313	8.06	0.125	0.33	0.069	9.17	6.24	2.08	0.154	0.18	0.178	0.005	6.96	0.229	0.029	52.76	16.68	2.05	0.34	30.33	0.00	32.72	22.39
3	MP19318	8.27	0.094	0.47	0.02	6.79	5.35	1.78	0.694	1.56	0.186	0.041	2.89	0.312	0.142	57.32	15.14	17.79	0.26	29.21	0.00	47.25	14.10
4	MP19324	8.22	0.13	0.46	0.062	9.43	6.04	2.25	0.423	0.21	0.207	0.002	7.34	0.189	0.021	50.78	14.83	2.40	0.36	28.14	0.00	30.89	23.60
5	MP19324	8.22	0.13	0.46	0.062	9.43	6.04	2.25	0.423	0.21	0.207	0.002	7.34	0.189	0.021	50.78	14.83	2.40	0.36	28.14	0.00	30.89	23.60
6	MP19324	8.22	0.13	0.46	0.062	9.43	6.04	2.25	0.423	0.21	0.207	0.002	7.34	0.189	0.021	50.78	14.83	2.40	0.36	28.14	0.00	30.89	23.60
7	MP19324	8.22	0.13	0.46	0.062	9.43	6.04	2.25	0.423	0.21	0.207	0.002	7.34	0.189	0.021	50.78	14.83	2.40	0.36	28.14	0.00	30.89	23.60
8	MP19329	8.34	0.073	0.63	0.025	8.55	6.16	2.14	0.272	0.16	0.2	0.002	6.98	0.215	0.013	51.58	15.70	1.82	0.20	27.36	0.00	29.39	26.19
9	MP19334	8.81	0.117	1.27	0.043	8.55	5.78	2.67	0.584	0.13	0.213	0.002	6.23	0.181	0.023	47.62	12.45	1.48	0.32	21.58	0.00	23.38	31.08
10	MP19334	8.81	0.117	1.27	0.043	8.55	5.78	2.67	0.584	0.13	0.213	0.002	6.23	0.181	0.023	47.62	12.45	1.48	0.32	21.58	0.00	23.38	31.08
11	MP19338	8.46	0.143	1.17	0.068	9.05	5.63	2.33	0.36	0.17	0.205	0.002	7.25	0.186	0.012	48.43	14.39	1.94	0.39	20.93	0.00	23.25	30.43
12	MP19338	8.46	0.143	1.17	0.068	9.05	5.63	2.33	0.36	0.17	0.205	0.002	7.25	0.186	0.012	48.43	14.39	1.94	0.39	20.93	0.00	23.25	30.43
13	MP19344	7.65	0.126	0.9	0.007	6	4.47	1.55	0.283	0.16	0.179	0.001	5.06	0.136	0.007	60.00	31.98	1.61	0.34	10.80	1.14	13.89	33.40
14	MP19344	7.65	0.126	0.9	0.007	6	4.47	1.55	0.283	0.16	0.179	0.001	5.06	0.136	0.007	60.00	31.98	1.61	0.34	10.80	1.14	13.89	33.40
15	MP19349	8.28	0.043	0.81	0.034	7.45	5.13	1.74	0.291	0.18	0.205	0.001	6.57	0.126	0.007	54.59	23.33	2.04	0.12	14.16	0.08	16.39	35.53
16	MP19349	8.28	0.043	0.81	0.034	7.45	5.13	1.74	0.291	0.18	0.205	0.001	6.57	0.126	0.007	54.59	23.33	2.04	0.12	14.16	0.08	16.39	35.53
17	MP19354	7.94	0.07	0.89	0.035	7.74	6.43	1.91	0.321	0.13	0.193	0.002	6.64	0.164	0.008	53.04	17.02	1.48	0.19	31.65	0.00	33.32	22.44
18	MP19354	7.94	0.07	0.89	0.035	7.74	6.43	1.91	0.321	0.13	0.193	0.002	6.64	0.164	0.008	53.04	17.02	1.48	0.19	31.65	0.00	33.32	22.44
19	MP19359	7.87	0.034	0.89	0.069	7.08	5.65	1.64	0.331	0.16	0.204	0.001	5.88	0.16	0.007	55.93	23.25	1.82	0.09	22.13	0.00	24.05	28.74
20	MP19365	8.41	0.116	0.68	0.023	7.38	7.03	1.7	0.269	0.21	0.195	0.001	6.15	0.155	0.006	53.50	14.30	2.40	0.32	35.62	0.00	38.33	22.91
21	MP19371	7.91	0.101	0.72	0.013	7.99	6.48	1.66	0.223	0.18	0.178	0.001	6.75	0.118	0.007	54.05	17.80	2.05	0.28	31.92	0.00	34.25	22.57
22	MP19382	7.74	0.066	0.9	0.031	7.74	6.27	1.27	0.168	0.16	0.192	0.002	7.2	0.134	0.005	54.79	20.29	1.82	0.18	28.50	0.00	30.50	25.63
23	MP19384	8.27	0.132	0.98	0.047	7.79	7	1.54	0.205	0.19	0.198	0.001	7.09	0.147	0.006	51.88	13.41	2.17	0.36	34.98	0.00	37.50	23.60
24	MP19386	8.75	0.122	0.76	0.003	7.71	6.15	2.04	0.241	0.18	0.194	0.002	6.8	0.151	0.012	51.69	15.36	1.95	0.33	24.82	0.55	27.65	30.13
25	MP19388	7.53	0.046	0.9	0.004	7.49	5.77	1.88	0.283	0.11	0.175	0.002	6.69	0.188	0.006	55.16	22.09	1.09	0.13	27.09	0.84	29.15	22.21

The results are presented as a csv file with a layout similar to the assay file.

Comet generates a Processing report for every job as a pdf file. The processing report includes a series of geochemical mineralogy diagrams coloured by the estimated mineral percentages which can be used to assess the plausibility of results. It also generates a series of plots which show potential mis-matches in results.

Measured vs Predicted Parity

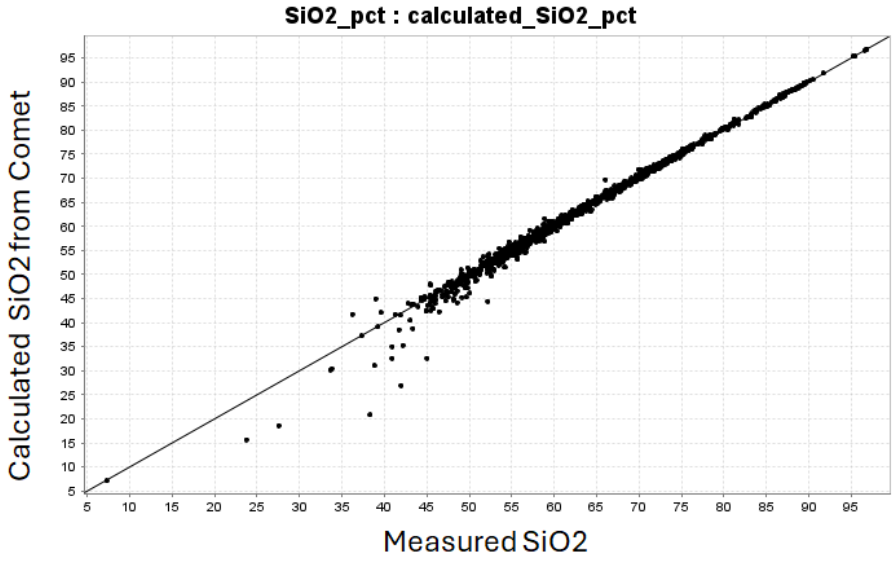


The report also generates a printout of the mineral list and compositions used in Comet for that calculation run.

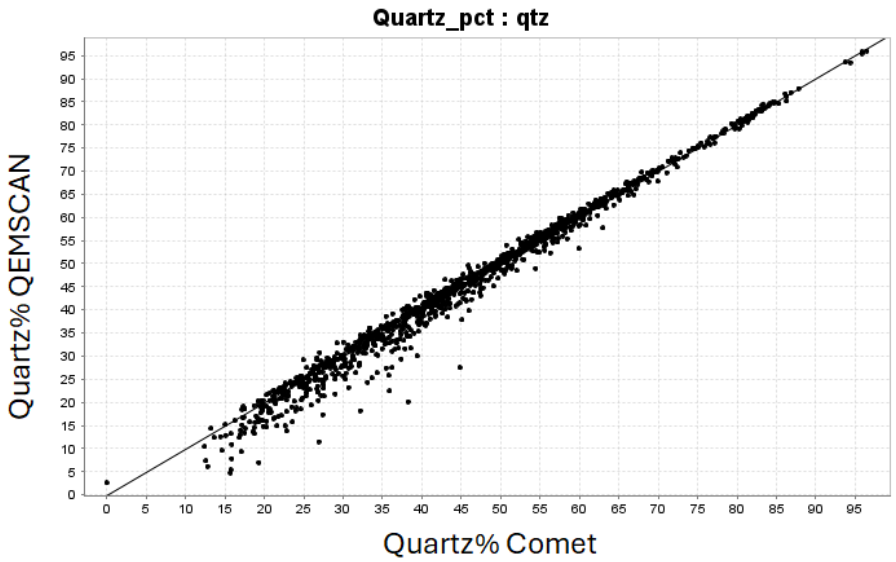
	Gibbs	Al	As	Ba	C	Ca	Cu	Fe	H	K	Mg	Mn	Na	OH	P	Pb	S	Si	Ti	Zn	O
Ankerite_SS	0.0	0.0	0.0	0.0	2.0	1.0	0.0	0.5	0.0	0.0	0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.00
Calcite	-3,0	0,0	0,0	0,0	1,0	1,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	3,00
Fe_Chlorite	-11,359	2,2	0,0	0,0	0,0	0,0	0,0	3,9	8,0	0,0	1,0	0,0	0,0	0,0	0,0	0,0	0,0	2,9	0,0	0,0	18,00
Mg_Chlorite	-15.742	2.2	0.0	0.0	0.0	0.0	0.0	1.0	8.0	0.0	3.9	0.0	0.0	0.0	0.0	0.0	0.0	2.9	0.0	0.0	18.00
Mn_Chlorite	-11.359	2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0	8.0	0.0	0.0	0.0	3.0	0.0	0.0	10.00
Kaolinite	-15,837	2,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	4,0	0,0	0,0	0,0	2,0	0,0	0,0	5,00
Albite	-14,5	1,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	1,0	0,0	0,0	0,0	0,0	3,0	0,0	0,0	8,00
Ba_Feldspar	-14.108	2.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	8.00
K_Feldspar	-14.108	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.0	0.0	0.0	8.00
Plagioclase_Basalt	-14,2	1,6	0,0	0,0	0,0	0,8	0,0	0,0	0,0	0,0	0,0	0,0	0,2	0,0	0,0	0,0	0,0	2,4	0,0	0,0	8,00
Rutile	-11,771	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	1,0	0,0	2,00
Apatite	-13.589	0.0	0.0	0.0	0.0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	4.0	0.0	0.0	0.0	0.0	0.0	12.00
Quartz	-14.985	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	2.00
Arsenopyrite	-0,954	0,0	1,0	0,0	0,0	0,0	0,0	1,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	1,0	0,0	0,0	0,0	0,00
Chalcopyrite	-1,062	0,0	0,0	0,0	0,0	0,0	1,0	1,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	2,0	0,0	0,0	0,0	0,00
Galena	-0.627	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.00
Pyrite	-1.2	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.0	0.0	0.0	0.00
Pyrrhotite	-1,5	0,0	0,0	0,0	0,0	0,0	0,0	1,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	1,0	0,0	0,0	0,0	0,00
Sphalerite	-2,468	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	0,0	1,0	0,0	0,0	1,0	0,00
Muscovite	-16.265	2.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9	0.0	0.0	0.0	2.0	0.0	0.0	0.0	3.1	0.0	0.0	10.00

How accurate are the results?

The best way to test the accuracy of Comet is to compare a data set with one of the “gold standard” methods, either qXRD or QEMSCAN. A comparison with QEMSCAN is shown here. I could take the assay results from the drill core and calculate mineralogy with Comet to compare with the QEMSCAN mineralogy from the same interval, but the QEMSCAN sample is usually not a one-to-one match with the assay interval. With every QEMSCAN sample, an XRF whole rock analysis is also measured. One of the issues with QEMSCAN is that this method also measures liberation of sulfide minerals from the silicate gangue, and to do that the average grain size of the prepared sample is much coarser that the pulverization that would be used to homogenize a sample prior to chemical analysis. A reconciliation is performed where a theoretical composition is computed from the measured percentages of minerals from the QEMSCAN raster and the assumed compositions of those minerals. The closest comparison is to compare measured QEMSCAN mineralogy with Comet mineral percentages calculated from the “computed” composition.

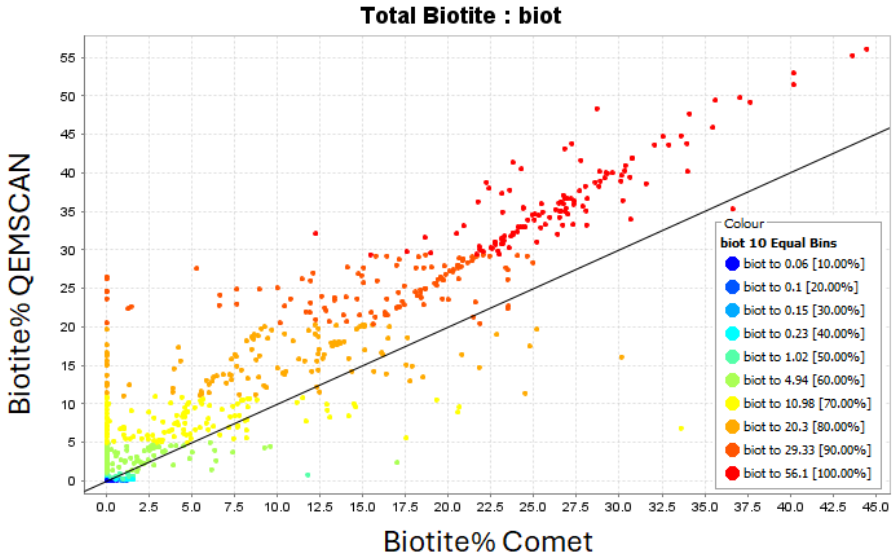


In this test, the measured SiO2 was not used in the calculations to replicate the results that might be generated from Comet using 4 acid digest ICP data. The SiO2 values back calculated from Comet are surprisingly accurate.

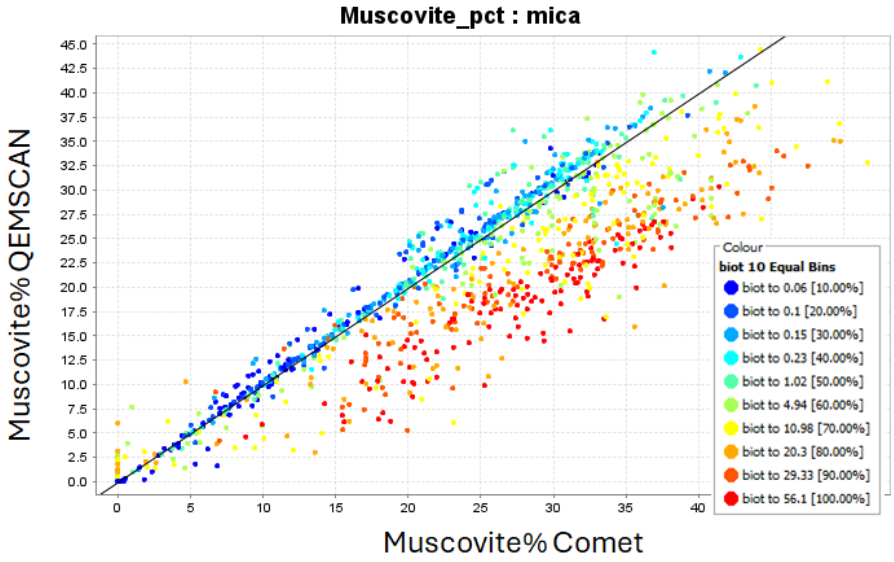


The comparison of measured versus calculated quartz looks good.

The comparison of measured versus calculated biotite highlights a problem with both QEMSCAN and qXRD. In this plot, there is a reasonable correlation between the QEMSCAN and Comet results, but there is a bias. The bias is due to the assumed composition of biotite used in the SIP (species identification protocol). It was assumed to be K(Fe,Mg)3AlSi3O10(OH)2. The spectral matching algorithm allows a significant degree of tolerance around this composition. Underlying the calculations in Comet, we have looked at a large number of published EMP biotite compositions, and the typical aluminium atoms per formula unit is usually closer to 1.4. The differences in the assumed biotite compositions accounts for the bias in this plot.



The comparison of measured versus calculated muscovite looks good for samples that do not have any biotite. For the biotite-rich samples, the nature of the mass balance calculation means that the differences in the biotite results have to be balanced out in the way K is assigned to other minerals.



Something that this comparison demonstrates is that the variability in solid solution compositions of white mica, biotite, chlorite, plagioclase and some carbonates is an issue for every quantitative mineralogy method, including the gold standard methods. One of the strengths of Comet is the measures we have taken to account for those solid solutions.

What are the sources of error?

Comet is a “normative” mass balance calculation. We start with more variables than constraints, which means there are an infinite number of mathematically possible solutions which we attempt to limit by imposing constraints. The biggest limitation is that with a 4-acid digestion method, we do not have analyses for Si, C and LOI.

The mass balance calculation requires that we start with a list of minerals and the compositions of those minerals. White mica, feldspar, chlorite, biotite and carbonates most notably are all solid solution minerals. The compositions of these minerals vary sample by sample. The methods within Comet attempt to account for the variability in these minerals, but it is still an approximation.

Our usual routine in Comet is to create a list of minerals for a deposit, however not every mineral is present in every sample. Missing minerals, or inclusion of minerals that are not present in a particular sample all introduce error.

The accuracy of Comet is highly dependent on the quality of the assay data. Under-reporting of aluminium from 4 acid digestion is a potential problem. This could be due to incomplete dissolution of aluminosilicate minerals or low recoveries due to the formation AlF_3.

Three minerals lying along a line or four minerals lying in a plane in multi-dimensional composition space are not independent end-members. For example, the method cannot successfully distinguish albite–anorthite mixtures from oligoclase–anorthite mixtures. Other examples of mineral mixtures that are difficult include assemblages with BOTH chlorite and biotite; plagioclase and epidote, muscovite-paragonite-albite and orthoclase. Other more specific examples of unsolvable mineral mixtures include overprints of kaolinite +/- montmorillonite on feldspar + mica bearing rocks.

If Comet is being used for defining domains in resource modelling, then we recommend that representative samples from those domains are tested with high precision mineralogic al techniques like QEMSCAN or qXRD.

References

Corbett, G.J. and Leach, T.M., 1998. *Southwest Pacific Rim gold-copper systems: structure, alteration, and mineralization*. Society of Economic Geologists.

Holland, T.J.B. and Powell, R.T.J.B., 1998. An internally consistent thermodynamic data set for phases of petrological interest. *Journal of metamorphic Geology*, *16*(3), pp.309-343