

Supplementary Information

4A Mathematica Code used for Developing Machine Learning Model

(* Predicting the weathering rates of minerals against a range of pH values *)

(* trainingData = {pH, Ca, Mg, Si, Na, Al, K, Fe, Ti, log k, E, nH+, WeatheringRate} *)

trainingData = {

{3, 0, 0, 3, 1, 1, 0, 0, 0, -10.2, 65, 0.46, -11}, (*Albite_Start*)

{3.5, 0, 0, 3, 1, 1, 0, 0, 0, -10.2, 65, 0.46, -11.2},

{4, 0, 0, 3, 1, 1, 0, 0, 0, -10.2, 65, 0.46, -11.4},

{4.5, 0, 0, 3, 1, 1, 0, 0, 0, -10.2, 65, 0.46, -11.6},

{5, 0, 0, 3, 1, 1, 0, 0, 0, -10.2, 65, 0.46, -11.8}, (*Albite_Finish*)

{3, 1, 0, 2, 0, 2, 0, 0, 0, -3.5, 16.6, 1.41, -7.5}, (*Anorthite_Start*)

{3.5, 1, 0, 2, 0, 2, 0, 0, 0, -3.5, 16.6, 1.41, -8},

{4, 1, 0, 2, 0, 2, 0, 0, 0, -3.5, 16.6, 1.41, -8.5},

{4.5, 1, 0, 2, 0, 2, 0, 0, 0, -3.5, 16.6, 1.41, -9}, (*Anorthite_Finish*)

{3, 0.5, 0, 2.5, 0.5, 1.5, 0, 0, 0, -5.85, 29.3, 1.02, -8.8}, (*Bytownite_Start*)

{3.5, 0.5, 0, 2.5, 0.5, 1.5, 0, 0, 0, -5.85, 29.3, 1.02, -9},

{4, 0.5, 0, 2.5, 0.5, 1.5, 0, 0, 0, -5.85, 29.3, 1.02, -9.2},

{4.5, 0.5, 0, 2.5, 0.5, 1.5, 0, 0, 0, -5.85, 29.3, 1.02, -9.4}, (*Bytownite_Finish*)

{3, 0.5, 0, 2, 0.5, 2, 0, 0, 0, -9.67, 65, 0.46, -10.6}, (*Oligoclase_Start*)

{3.5, 0.5, 0, 2, 0.5, 2, 0, 0, 0, -9.67, 65, 0.46, -10.8},

{4, 0.5, 0, 2, 0.5, 2, 0, 0, 0, -9.67, 65, 0.46, -11},

{4.5, 0.5, 0, 2, 0.5, 2, 0, 0, 0, -9.67, 65, 0.46, -11.2}, (*Oligoclase_Finish*)

{3, 0, 0, 3, 0, 1, 1, 0, 0, -10.1, 51.7, 0.5, -11}, (*K-Feldspar_Start*)

{3.5, 0, 0, 3, 0, 1, 1, 0, 0, -10.1, 51.7, 0.5, -11.3},

{4, 0, 0, 3, 0, 1, 1, 0, 0, -10.1, 51.7, 0.5, -11.6},

{4.5, 0, 0, 3, 0, 1, 1, 0, 0, -10.1, 51.7, 0.5, -11.9},

{5, 0, 0, 3, 0, 1, 1, 0, 0, -10.1, 51.7, 0.5, -12.2}, (*K-Feldspar_Finish*)

{3, 3, 0, 3, 0, 0, 0, 2, 0, -5.2, 94.4, 1, -7.2}, (*Andradite_Start*)

{3.5, 3, 0, 3, 0, 0, 0, 2, 0, -5.2, 94.4, 1, -7.8},

{4, 3, 0, 3, 0, 0, 0, 2, 0, -5.2, 94.4, 1, -8.4},

{4.5, 3, 0, 3, 0, 0, 0, 2, 0, -5.2, 94.4, 1, -9},

{5, 3, 0, 3, 0, 0, 0, 2, 0, -5.2, 94.4, 1, -9.6}, (*Andradite_Finish*)

{3, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -7}, (*Fayalite_Start*)

{3.5, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -7.5},

{4, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -8},

{4.5, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -8.5},

{5, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -9},

{5.5, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -9.5},

{6, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -10},

{6.5, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -10.5},

{7, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -11},

{7.5, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -11.5},

{8, 0, 0, 1, 0, 0, 0, 2, 0, -4.8, 94.4, 1, -11.8},

(*Fayalite_Finish*)

{3, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -7.4},

(*Forsterite_Start*)

{3.5, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -7.7},

{4, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -8},

{4.5, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -8.3},

{5, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -8.6},

{5.5, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -8.9},

{6, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -9.2},

{6.5, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -9.5},

{7, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -9.8},

{7.5, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -10.1},

{8, 0, 2, 1, 0, 0, 0, 0, 0, -6.85, 67.2, 0.47, -10.4},

(*Forsterite_Finish*)

{3, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -8.3},

(*Augite_Start*)

{3.5, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -8.6},

{4, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -8.9},

{4.5, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -9.2},

{5, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -9.5},

{5.5, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -9.8},
{6, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -10.1},
{6.5, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -10.4},
{7, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -10.7},
{7.5, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -11},
{8, 0.5, 0.25, 1, 0.5, 1.25, 0, 0.25, 0.25, -6.82, 78, 0.7, -11.2},

(*Augite_Finish*)

{3, 0, 2, 2, 0, 0, 0, 0, 0, -9.02, 80, 0.6, -10},
{3.5, 0, 2, 2, 0, 0, 0, 0, 0, -9.02, 80, 0.6, -10.3},
{4, 0, 2, 2, 0, 0, 0, 0, 0, -9.02, 80, 0.6, -10.6},
{4.5, 0, 2, 2, 0, 0, 0, 0, 0, -9.02, 80, 0.6, -10.9},
{5, 0, 2, 2, 0, 0, 0, 0, 0, -9.02, 80, 0.6, -11.2},
{5.5, 0, 2, 2, 0, 0, 0, 0, 0, -9.02, 80, 0.6, -11.5},
{6, 0, 2, 2, 0, 0, 0, 0, 0, -9.02, 80, 0.6, -11.8},
{6.5, 0, 2, 2, 0, 0, 0, 0, 0, -9.02, 80, 0.6, -12.1},

(*Enstatite_Finish*)

{3, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -6.5},
{3.5, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -6.7},
{4, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -6.9},
{4.5, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -7.1},
{5, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -7.3},
{5.5, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -7.5},
{6, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -7.7},

(*Wollastonite_Start*)

{6.5, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -7.9},
{7, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -8.1},
{7.5, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -8.3},
{8, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -8.5},
{8.5, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -8.7},
{9, 1, 0, 1, 0, 0, 0, 0, 0, -5.37, 54.7, 0.4, -8.9}

(*Wollastonite_Finish*)

{3, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -7.3},
{3.5, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -7.7},
{4, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -8.1},
{4.5, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -8.5},
{5, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -8.9},
{5.5, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -9.3},
{6, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -9.7},
{6.5, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -10.1},
{7, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -10.5},
{7.5, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -10.9},
{8, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -11.3},
{8.5, 0, 3, 2, 0, 0, 0, 0, 0, -5.7, 75.5, 0.8, -11.7}

(*Lizardite_Start*)

(*Lizardite_Finish*)

};

(* Define Regression Models Random Forest for log k, E, nH+, Weathering Rate *)

```
logkModel = Predict[trainingData[[All, {1,2,3,4,5,6,7,8,9}]]->trainingData[[All,10]],Method->"RandomForest"];
```

```
AEModel = Predict[trainingData[[All, {1,2,3,4,5,6,7,8,9}]]->trainingData[[All,11]],Method->"RandomForest"];
```

```
ROModel = Predict[trainingData[[All, {1,2,3,4,5,6,7,8,9}]]->trainingData[[All,12]],Method->"RandomForest"];
```

```
WeatheringRateModel = Predict[trainingData[[All, {1,2,3,4,5,6,7,8,9}]]->trainingData[[All,13]],Method->"RandomForest"];
```

```
(* Synthesized mineral *)
```

```
newData = {3, 2, 1, 2, 0, 0, 0, 0, 0};
```

```
predictedWeatheringRate = model[newData]
```

```
(* Predict log k, E, nH+, Weathering rate *)
```

```
logk = logkModel[newData];
```

```
AE = AEModel[newData];
```

```
RO = ROModel[newData];
```

```
WeatheringRate = WeatheringRateModel[newData];
```

```
(*Print the Results*)
```

```
Print["log k = ", logk];
```

```
Print["E = ", AE];
```

```
Print["nH+ = ", RO];
```