

Error Propagation in Aqueous Equilibrium Calculations

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Error analysis calculates the propagation of errors in the input variables to the error in each output variable and determines what fraction of output error is caused by each input error. This is very useful in planning experiments and analysing calculations. For example, in calculating the solubility of CaCO₃ at a given pH and temperature, the possible errors in controlling or measuring pH and temperature can be used to calculate the expected error in solubility. Propagation of errors in the thermodynamic parameters can also be included in the analysis.

In another example, data on Jarosite solubility (Baron et al., 1996) is analysed to obtain a 95% confidence limit on Jarosite Log(Ksp) based on reported concentration and pH.

Monte Carlo simulations produced the same 95% confidence limits as this new procedure but did not provide information about the importance of each input error. This new procedure calculates what fraction of the output error is the result of each input error.

I used the Environmental Simulation Program from OLI Systems for this analysis. Other equilibrium calculation codes that use the Newton-Raphson solution technique could also be used.

Baron D, & Palmer CD, *Geochimica et Cosmochimica Acta*, **60**, 185-195, (1996).