Advances in geochemical modeling applied to the characterization and remediation of acid mine drainage

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At the start of my PhD work, aqueous speciation codes were in their infancy (WATEQ, REDEQL, PATHCALC). Using the WATEQ code, I found a quantitative Nernstian correlation between measured and calculated redox potentials (Eh) for acid mine waters. This result was one of the first to show the reliability of our speciation calculations. The codes WATEQ have evolved to WATEQ4F, and REDEQL to MINTEQA2. Current popular codes are PHREEQC, EQ3/6, TOUGHREACT, and The Geochemist's Workbench®.

More recently, pyrite oxidation can be simulated and portrayed graphically and the results match field data well. Through modeling water chemistry data, we can now draw quantitative generalizations about the behavior of iron and aluminum during the oxidation and neutralization of acid mine drainage. These generalizations are a key to understand how other trace elements will behave, including ore-forming processes during weathering of sulfides. USGS researchers have shown that after calibrating stream characteristics through tracer-injection studies with synoptic sampling, it is possible to estimate the downstream water chemistry after implementing different remedial options to optimize the most cost-effective solution. Today's researchers and consultants can model reactive-transport of fluid flow through tailings, waste-rock piles, open pits, and the fate of mine contaminants in receiving streams. Our modeling has become more sophisticated than the actual field data which is needed to constrain the models. Meaningful predictions necessitate the modeler to have a knowledge of all the model assumptions, the complexities of hydrogeology, and of mineral-water reactions to know the range of computational uncertainties. Consequently we have seen predictions and modeling scenarios that may bear little resemblance to the real situation. Predicting the potential for acid production from a new mining operation is not simple and requires collection of key hydrogeochemical information in addition to engineering tests (AP/NP, ABA, HCT). More work is warranted on monitoring remediated sites and testing predictions with measurements made over the course of many years. The path to improved modeling with hypogene or supergene ore formation and weathering of mine wastes is through continual testing of predictions with carefully collected field data.