Aqueous Geochemical Modeling to Evaluate Metal-Laden Discharges from Coal Mines

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User-friendly aqueous geochemical tools have been developed with PHREEQC [1] that combine rate models for gas exchange, limestone dissolution, and iron oxidation plus reactions with chemical neutralizing or oxidizing agents to simulate changes in water quality during treatment of net-acidic or net-alkaline iron-laden effluent. The limestone kinetics tool utilizes an established rate model for calcite dissolution and precipitation [2]; the rate expression considers solution chemistry, mainly pH and partial pressure of CO_2, plus the surface area and purity of limestone particles. The iron-oxidation kinetics tool utilizes established rate models for the oxidation of aqueous Fe(II), which depends on dissolved O_2 and pH [3, 4, 5]. The Fe(II) oxidation rate combines abiotic homogeneous and heterogeneous rate laws, which indicate a positive relation with pH from 5 to 8, plus a generalized microbial oxidation rate, which indicates a negative relation with pH from 5 to 2.8. A first-order rate law describes O2 ingassing and CO2 outgassing as the dissolved gases approach atmospheric equilibrium. Sequential treatment steps that have different detention time, aeration rate, limestone quantity, Fe(III) solids, and temperature can be simulated. A user interface facilitates input of initial water chemistry and adjustment of kinetic variables. Graphical and tabular output indicates the changes in pH and solute concentrations in treated effluent as a function of detention time, plus the cumulative quantity of precipitated solids. By adjusting kinetic variables or chemical dosing, various passive and/or active treatment strategies can be identified that achieve the same desired effluent quality. Cost analysis software such as AMDTreat [6] can then be used to evaluate the cost-effectiveness and feasibility for installation and operation of those equally effective treatments.

[1] Parkhurst and Appelo (2013) *USGS Tech. Methods* 6-A43; [2] Plummer et al. (1978) *Am. J. Sci.* 278, 179-216; [3] Cravotta (2015) *Appl. Geoch*. 54, 223-251; [4] Dempsey et al. (2001) *Geoch. Explor. Env. Anal.* 1, 81-88; [5] Kirby et al. (1999) *Appl. Geoch.* 14, 511-530; [6] Cravotta et al. (2015) *Mine Water Environ.* 34, 136-152.