A GEOCHEMICAL KINETICS MODULE FOR AMDTreat TO ESTIMATE THE EFFECTS OF AERATION ON RATES OF DECARBONATION AND IRON OXIDATION[1]

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Abstract: A new PHREEQC "kinetics tool" has been developed for the AMDTreat computer program that utilizes established rate equations for gas exchange and pH-dependent oxidation of dissolved ferrous iron (aqueous Fe(II)). The kinetic model accurately simulates the interdependent effects of CO_2 outgassing (decarbonation), O_2 ingassing, and pH on Fe(II) oxidation rates for net-alkaline or net-acidic mine drainage. A first-order asymptotic rate law is used to simulate the rates of CO_2 outgassing and O_2 ingassing, which result as the dissolved gases in groundwater that is retained in ponds or wetlands gradually equilibrate with the atmosphere or undergo rapid exchange due to aggressive pre-aeration or other forms of aeration. Aeration promotes CO_2 outgassing, thereby increasing pH and the rate of Fe(II) oxidation. The rate of Fe(II) oxidation is estimated by using the combined homogeneous and heterogeneous rate laws plus a generalized microbial oxidation rate, which becomes relevant at low pH (< 5). The homogeneous rate law indicates the rate of Fe(II) oxidation increases 100-fold when pH increases by 1 unit at pH 5-8 and dissolved O_2 concentration is constant. The additional heterogeneous rate law quantifies the potential catalytic effects of suspended Fe(III)-oxide particles on Fe(II) oxidation and, thus, permits the evaluation of sludge recirculation on iron-removal efficiency. From pH 2.8 to approximately pH 5, Fe(II) oxidation rates are negatively correlated with pH and proportional to the concentration of iron-oxidizing bacteria. Temperature correction is applied to the gas solubility and gas-exchange rates and to the Fe(II) oxidation rate constants. The kinetics tool permits a user of AMDTreat to select among a range of values for the O_2 ingassing and CO_2 outgassing rates, the iron oxidation rate constants, the concentration of Fe(III) in recirculated solids, and the "most probable number" of iron-oxidizing microbes. The selectable gas-exchange rates generally correspond to specific aeration technologies that may be incorporated at passive and active treatment facilities. Each technology has different potential costs for installation and operation, which are computed by AMDTreat, depending on the size and/or number of aeration technologies and energy usage. The kinetic simulations for the specified initial water quality and treatment conditions indicate changes in the pH, dissolved iron, alkalinity, and other solute concentrations remaining in treated effluent at progressive elapsed times (retention time), plus the cumulative quantity of precipitated solids produced by treatment. AMDTreat uses this information to compute the estimated volume and associated cost for removal of the resultant sludge, which contains the precipitated solids.

Additional Key Words: Mine water treatment, PHREEQC, geochemical model, cost analysis

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