Modeling the Effects of Mass Transfer Limitations in Limestone-Based Passive Treatment Systems[1]

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Abstract: A growing body of evidence suggests that the rates of limestone dissolution and metal hydroxide precipitation in limestone-based passive treatment systems such as open limestone channels or anoxic limestone drains are governed by mass transfer phenomena at the water-rock interface. Because mass transfer limited reaction rates respond not only to the chemical composition of the water but also to local velocity fields and to the physical geometry of the rock, this introduces substantial complexity into the task of predicting treatment system performance either on the basis of process modeling or scale-up of bench-top experiments. In this paper, we couple the geochemical modeling tool, PHREEQC, with mass-transfer correlation theory developed in the contaminant hydrogeology community to explore the potential effects of mass transfer phenomena on pH evolution, alkalinity generation, and metals precipitation during treatment. We present our modeling results in comparison to data collected in both lab- and field-scale systems but we also use the model to introduce the range of phenomenological responses that could arise due to mass transfer limitation. From a design perspective, the effects of local velocity on mass transfer rate presents not only a challenge to predictive modeling but also an opportunity for design optimization. This type of opportunity has been previously exploited in permeable reactive barriers for groundwater remediation by introducing funnel-and-gate structures to achieve optimal flow velocity. In the mine drainage context, mass transfer optimization could be achieved by a mix of limestone size selection and overall system dimensions. We use the model described above to explore the nature of this optimization problem.

Additional Key Words: dissolution, precipitation, reaction rate.

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3. Work reported here was conducted near 40.5601° N, 78.5486° W