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A three-dimensional hydro-geochemical model to assess lake acidification risk☆

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ABSTRACT

Biogeochemical and hydrological fluxes from riparian zones to lake environments can be significant, particularly for shallow systems experiencing large variations in water level, yet they are not considered in water quality models. To address this challenge we dynamically coupled a three-dimensional surface water model with a soil hydro-geochemical model of the riparian zone and used the coupled system to simulate the impacts of acid sulfate soils on the water quality of a morphologically complex coastal lake system in South Australia. A 3-yr simulation was undertaken to capture a period of exposure and re-flooding of pyrite-bearing sediments and acid fluxes to the lake. Model performance was assessed against data from several acidification events that occurred and the simulations reproduced the observed spatio-temporal variation in the expression of soil and water acidity. The model approach introduced here has potential for simulating systems where the terrestrial–aquatic linkage is important in shaping water quality.

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Software availability

Name of software: ELCOM-CAEDYM + ASS (Acid Sulfate Soils)
Developers: Centre for Water Research, University of Western Australia
Availability and Online Documentation: Download and manual for ELCOM-CAEDYM from: http://www.cwr.uwa.edu.au/software1/downloads/policy.php
Email: matt.hipsey@uwa.edu.au for the ASS plugin module.
Hardware required: Any
Software required: MS Windows or Linux
Programming language: Fortran90

1. Introduction

Potential acid sulfate soils (PASS) accumulate naturally in anaerobic lake sediments and saturated soils where there is sufficient supply of sulfate, organic matter, and iron minerals (Dent and Pons, 1995). Under reducing conditions sulfate is bacterially reduced to sulfide, which reacts with reduced iron to form iron sulfide minerals, typically pyrite (FeS_2). These sulfide minerals are generally stable under reducing waterlogged conditions and pose no environmental risk. However, if they are exposed to air, the pyrite can oxidize to generate large amounts (tens to hundreds of mol H^+/tonne in some circumstances) of acidity in the sediment (e.g., Cook et al., 2004; Fitzpatrick et al., 2010), which may then be referred to as actual acid sulfate soils (AASS). If severe sulfuric acidic conditions develop in the soil (pH < 4), weathering of alumino-silicate (e.g. clay) minerals is enhanced resulting in high concentrations of soluble aluminum (Ferguson and Eyre, 1999). Precipitation of secondary acidic minerals (e.g., jarosite) may also occur. The rewetting of acid sulfate soils can mobilize acidity and metals into the water column (Sundström et al., 2002; Simpson et al.,

☆ Thematic Issue on Aquatic ecosystem models.

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2010) and result in water body acidification and severe ecological impacts (Ward et al., 2004a; Sammut et al., 1995).

Recently, Australia's largest river system, the Murray–Darling Basin, experienced the worst drought conditions and lowest flows in over 100 years of records (Leblanc et al., 2012). This resulted in severe water quality impacts in the Lower Lakes of South Australia with greatly increased salinity, eutrophication, and turbidity (Mosley et al., 2012). Of additional concern was the rapid rate of water level decline exposing perimeter regions of the pyrite-bearing lake sediment to the atmosphere and resulting in acid generation (Fitzpatrick et al., 2009). The unprecedented environmental change that occurred made the consequences difficult to predict and therefore manage. Potential impacts of concern were possible deleterious effects on lake ecology, including damage of substantial area of wading waterbird habitat, risks of elevated metal concentrations in drinking water offtakes, and the potential for a catastrophic ecosystem shift due to system-wide acidification.

The high costs, long lead times, and uncertainty of success in designing and implementing management interventions to prevent and/or manage acidification, provided motivation for the development of quantitative modeling tools to assess risks and test scenarios. Specific requirements for a model were to dynamically assess: 1) the effect of changing water balance over the lake, leading to decrease in lake levels, 2) the associated degree of partial saturation in adjacent pyrite-bearing sediments (and hence the rate of oxygen ingress and pyrite oxidation), which is a function of the texture of the sediments, 3) the initial amount of pyrite present in exposed sediments with associated acidity generation over time during oxidation, 4) acid attenuation by reactions such as carbonate dissolution and anaerobic sulfate reduction; 5) the pathways of transport of acidity from exposed acidic sediments to the lake (e.g. transport of acidity from the unsaturated to the saturated zone via percolation, lateral groundwater transport into the lake, flushing of the acidified sediments caused by wind-driven lake seiching, and diffusion during sediment re-inundation); and 6) the fate of acidity once in the lake, including neutralization and mixing processes. Quantifying these complex controls on acid generation, transport, and attenuation thus required detailed consideration of physical processes in soils and surface waters, as well as biogeochemical sources and sinks.

Modeling tools exist for studying individual parts of an acid sulfate soil-riparian zone-lake system. For example the hydrodynamics and water quality of lakes (Chung et al., 2009; Kara et al., 2012), the hydrology and geochemistry of variably saturated soils (Mayer et al., 2002; Simunek et al., 2008), and groundwater physical–geochemical dynamics (e.g., Prommer et al., 2000). However there was no obviously suitable platform to integrate these components in order to assess the risk that acid sulfate soil exposure could result in lake acidification, and which was suited to assess the range of management scenarios being considered across a large spatial area. Models that have previously been developed to specifically look at acid sulfate soils focus on the geochemical processes in the soil and shallow groundwater. For example, a 1-D acid sulfate soil model (SMASS) was used to assess agricultural drainage impacts in heavy clay soils with macropore-dominated oxygen transport (Bronswijk and Groenenberg, 1992; Bronswijk et al., 1993, 1995). This model was later applied in conjunction with 3-D groundwater model for assessing water management strategies (Blunden and Indraratna, 2000; Indraratna et al., 2001). Similar principles were incorporated into ACID3D (Blunden and Indraratna, 2001), which was then used to investigate coastal drain management. Cook et al. (2004) developed a steady state 1-D model to be used in conjunction with soil pore gas measurements (O_2 and CO_2) to estimate competing rates of oxygen consumption by pyrite and organic matter oxidation, and the resulting acidity generation. In the parallel field of quantifying acid mine drainage (AMD) generation, many modeling studies have quantified pyrite oxidation and other reactions in porous media (e.g., Jaynes et al., 1984; Davis and Ritchie, 1986; Elberling et al., 1994; Scharer et al., 1994; Lichtner, 1996; Wunderly et al., 1996; Mayer et al., 2002; Salmon and Malmstrom, 2004). However, the existing models for acid sulfate soils and AMD do not consider the connection, and potential feedback of, the hydrodynamics of adjacent surface water bodies on acid sulfate soil processes.

The impact of acid drainage on surface waters has been modeled in water bodies formed in mining voids upon groundwater rebound (pit lakes) or natural lakes receiving AMD (Davis et al., 2006; Moncur et al., 2006; Bozau et a., 2007; Castendyk and Webster-Brown, 2007; Oldham et al., 2009). In these studies, vertical and lateral movement of water in the lake (e.g., seiching and water level fluctuations) is not linked to generation and transport of acidity in adjacent sediments, but rather they have received acidity inputs as an external boundary condition. Models have also been developed for determining lake acidification risks following acid rain deposition in the northern hemisphere (Larssen et al., 2003; Dennis et al., 2005) and potential impact of acidic conditions on pit lake nutrient cycling (Oldham et al., 2009), however, these have not considered the many processes relevant to acid sulfate soils such as pyrite oxidation on exposed marginal sediments.

In this paper the development of a novel hydro-geochemical model is reported and used to assess lake acidification risk as water level decline exposed pyrite-bearing lake sediments. The model connects a spatially-resolved conceptual model of soil physical and geochemical processes with a 3-D surface water hydrodynamic–biogeochemical model (ELCOM–CAEDYM), and is suited to simulate lake water quality over time-scales of multiple years, relevant to the management actions being considered. Model predictions are assessed against a substantial field data set collected over the period from January 2008 to December 2010 in the Lower Lakes and used to quantify the pathways of acidity generation and attenuation and subsequent water quality response. A range of forecast flow and water level management scenarios are also run to identify 'hotspots' of acidification risk and estimate system 'tipping points'. Results from the model are used to inform management actions and development of environmental flow policy for the region. The model has broad relevance to other locations that may experience similar events in the future due to climatic or hydrological changes.

2. Model development

2.1. Existing hydrodynamic and biogeochemical model description

The model for assessing acidification risk was developed by coupling an existing lake hydrodynamic–water quality model (ELCOM–CAEDYM) to a model able to resolve the basic hydrology and biogeochemistry of exposed acid sulfate soil material. The 3-D Estuary, Lake and Coastal Ocean Model (ELCOM) is used to predict the hydrodynamics, temperature and salinity distribution of the lake domain in response to environmental forcing (Chung et al., 2009). The Computational Aquatic Ecosystem Dynamics Model (CAEDYM) is coupled to ELCOM to simulate numerous biogeochemical processes and parameters including: inorganic particles, oxygen, organic and inorganic nutrients (C, N, P and Si), and chlorophyll-a (e.g., Leon et al., 2012). CAEDYM also includes a geochemistry module designed to solve the equilibrium speciation of geochemical components (including Al, Ca, Mg, Na, K, Fe(II), Fe(III), Mn(II), SiO_2, Cl, DIC, SO_4, PO_4, NO_3, and NH_4), including precipitation/dissolution of several mineral phases ($Fe(OH)_3$, $Al(OH)_3$, MnO_2 and $CaCO_3$) and kinetic processes (e.g. microbially-

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