Water Quality Modeling of Pit Lakes: Development of a Multiply-Coupled Groundwater Lake Circulation and Chemical Model

Mike Müller [a)], Florian Werner [b)], Katja Eulitz [b)], Bastian Graupner [b)]

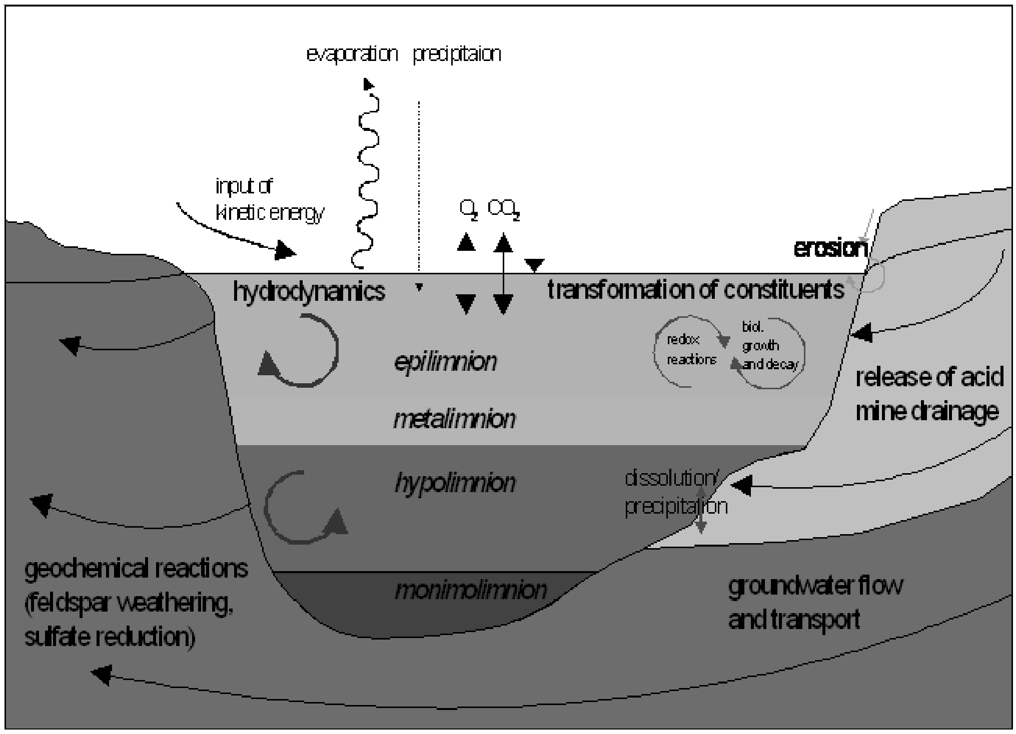
[a)] *Ingenieurbüro für Grundwasser GmbH, Nonnenstr. 9, 04229 Leipzig, Germany*
e-mail: m.mueller@ibgw-leipzig.de
[b)] *Dresdner Grundwasserforschungszentrum e.V., Meraner Str. 10, 01217 Dresden, Germany*

Abstract
Water quality of pit lakes is often determined by acid mine drainage. The system is complex because flow processes in the groundwater and the lake as well as chemical and biological water quality processes influence each other. Modeling has to consider all of these processes with their feedback to achieve reasonable representation of the system. The modeling system, MODGLUE, couples the existing groundwater model PCGEOFIM, the lake model CE-QUAL-W2, and the hydrochemical model PHREEQC. All important processes and their feedback loops are included in the model. It has been successfully applied to several lakes in Germany and is being further developed.

Key words: water quality modeling, acid mine drainage, coupled modeling, lake modeling, groundwater water modeling, pit lakes, MODGLUE, PCGEOFIM, CE-QUAL-W2, PHREEQC

Introduction
Modeling of pit lake water quality is a sophisticated task that typically involves processes that are investigated in different scientific fields. Figure 1 gives an overview of important processes in acidic pit lakes. Often pit lakes are fed by groundwater that may carry considerable amounts of acid mine drainage (AMD). Other sources of acidity are erosion materials from banks transported by rain water or mobilized by wind waves. Circulation processes in the lake are driven by wind and influenced by temperature- and possibly concentration-caused stratification. Water quality in the lake is determined by chemical reactions and biological processes such as algal growth and nutrient cycles. All of these processes interact with each other, forming a complex feedback system.

***Figure 1** Important processes in acidic mining lakes*



In order to model this system, modeling knowledge from different scientific domains such as groundwater, lake circulation, hydrochemistry, and limnology needs to be combined. The modeling system MODGLUE couples the groundwater flow and transport model PCGEOFIM with the lake circulation water quality model CE-QUAL-W2 and the hydrochemical model PHREEQC. In addition, a simple erosion model provides AMD inputs from banks. Another feature of MODGLUE is the possibility to model the adding of substances to the lake. This allows one to model oxygen addition to the hypolimnion or chemical treatment of lake water to neutralize it.

Groundwater Model: PCGEOFIM

PCGEOFIM (Sames et al., 2005; Müller et al., 2003) is a finite volume groundwater flow and transport model that was specifically designed for mining and post-mining areas more than 35 years ago. It provides some special features to account for mining-specific conditions. Subsurface parameters can be specified as time-dependent allowing for modeling of excavation of mine pits, filling with overburden, and creation of lakes, all in one model run. While working with a regular grid, multiple nested grid refinements that may overlap can be used to get higher resolution in regions of special interests. The model offers many ways to specify groundwater recharge such as keeping it constant over time, having it depend on groundwater levels, or getting it from a sophisticated coupling with a rainfall-runoff-soil-water-budget model.

PCGEOFIM provides a simple yet very useful mechanism to account for the interactions between lakes and groundwater. The lake is represented as a water level volume relationship, budgeting all in- and out-flows, such as groundwater and rivers. Precipitation and evaporation yields a new lake water volume and hence a new water level. This water level is used as the head for Cauchy boundary conditions that act jointly as “the lake”. Rivers can also be represented by several Cauchy boundary conditions that act jointly while the discharge is calculate by Manning’s formula. Many special boundary conditions, such as vertical and horizontal multi-level wells, defined outflow levels of lakes as well as sophisticated connections between rivers, lakes, and pipelines with control mechanisms can be used to provide a high level of representation of the real system.

Lake Model: CE-QUAL-W2

CE-QUAL-W2 (Cole and Buchak, 2005) is a two-dimensional finite difference model for lakes and reservoirs that calculates flow, transport, and limnological water quality. It solves the Navier-Stokes-Equation with a large eddy diffusion approach, accounting for kinetic energy introduced by wind and density-driven flow determined by temperature and solution concentrations. It is widely used to model lake stratification and water quality of lakes, reservoirs, and rivers all over the world. PSU (2008) lists about 2400 of its applications worldwide. Many water-quality determining processes, such as algal growth, nutrient cycle, and oxygen concentration can be modeled. However, it describes inorganic chemical processes insufficiently for modeling AMD effects.

Hydrochemical Model: PHREEQC

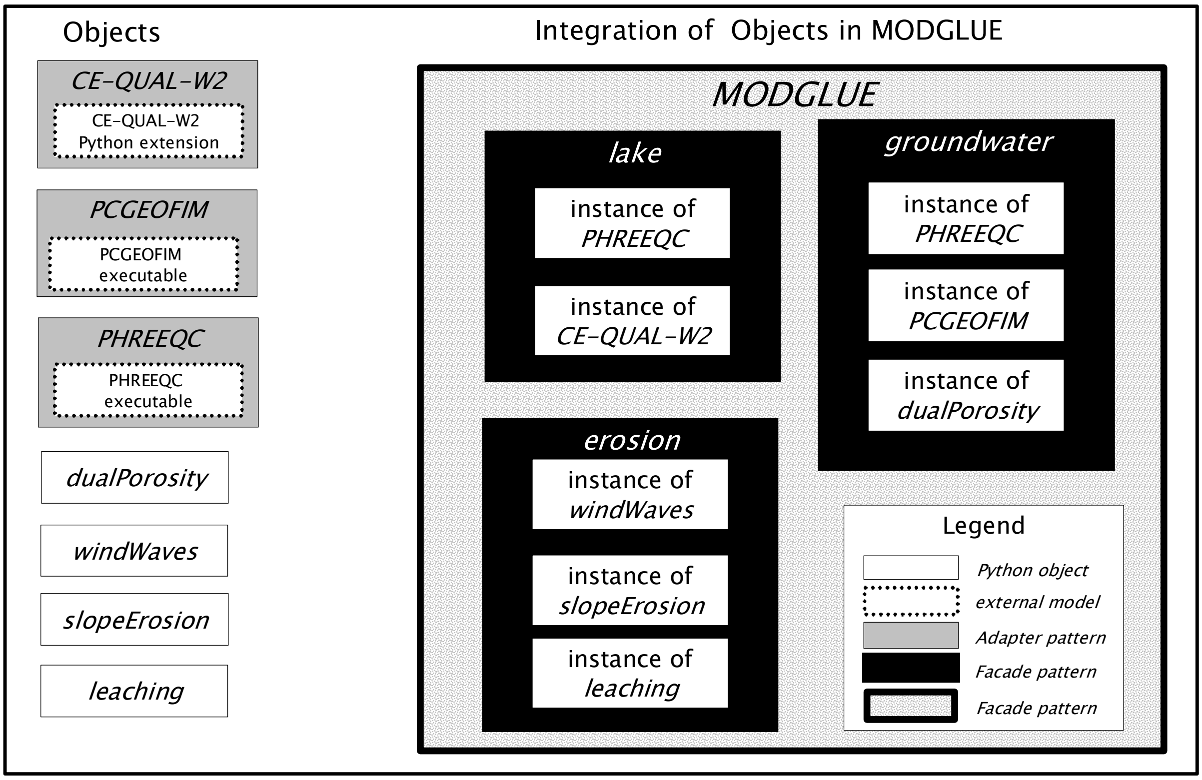
PHREEQC (Parkhurst and Appelo, 1999) is probably the most widely used hydrochemical model that allows one to represent a wide range of chemical reactions. Nearly all inorganic and organic chemical reactions can be modeled with the help of its built-in programming language.

Coupled Model: MODGLUE

The development of MODGLUE, which stands for *MOD*el for Prediction of *G*roundwater and Erosion influenced *L*ake Water Quality *U*sing *E*xisting Models, started in 2000 (Müller, 2004). The coupled model includes spatially distributed exchange of water flow and flux between groundwater and lake, limnological and chemical water quality changes as well as effects of eroded materials on water quality. The model is capable of representing all major influences on water quality and their interactions, as shown in Figure 1. It has been successfully applied to several lakes in Germany for prediction of water quality and evaluation of effects of lake treatments. The water quality of the pit lake Bärwalde has been predicted (Müller and Werner, 2004; Werner et al., 2008). A new groundwater model capable of density-driven flow MODMST (Boy, 2001) has been coupled to MODGLUE and used for water quality modeling of Lake Großkayna (Müller and Werner, 2003). Deep water aeration has been incorporated into the model with a new source-sink term that adds or subtracts substances at a given location with a provided schedule. Water quality predictions were conducted at other lakes in the central German mining region including Lake Zwenkau, Lake Bockwitz, and Lake Hain (Müller, 2005). For this, the model was again modified to allow treatment of acidic lake water with alkaline substances.

Figure 2 shows the architecture of MODGLUE. On the left, the objects, designed with object-oriented programming techniques, are depicted. The existing models were wrapped with help of the Python programming language, applying the adapter pattern; this was then used as a component for MODGLUE, applying the façade pattern. This leads to a flexible setup, facilitating understanding and extension of the system.

Figure 2 *Schematic of the architecture of the modeling system MODGLUE*



Conclusion

The approach of coupling existing models and incorporating them in one program was successful. All important processes for acidic lakes are represented in MODGLUE. The flexible setup of the system, using techniques from software engineering, helps one to understand the complex program and to extend it to different requirements at different sites. Application of the model to different lakes resulted in predictions of lake water quality as well as effects of different lake water treatments.

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