A COUPLED HYDRODYNAMIC-GEOCHEMICAL MODEL OF MEROMICTIC PIT LAKE WALDSEE

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ABSTRACT

Pit lakes are known for their tendency to become meromictic. Biogeochemical reactions are one potential reason. In these cases, lake hydrodynamics is controlled by lake water biogeochemistry. Most of the existing numerical stratification models for lakes calculate the chemical composition separately from hydrodynamic and transport calculations. However, if the geochemistry controls the stability of the stratification, temperature profiles cannot be predicted accurately without considering geochemical transformations in the hydrodynamic model.

We included a new density method which couples hydrodynamics and hydrogeochemistry by accounting for a chemical connection term in the calculation of water density. Such connection term depends on the chemical water composition. The UNESCO (1983) equation commonly used to calculate water density has been replaced with a new density equation based on Chen & Millero (1986) which has a weighting factor accounting for the water chemical composition. It is shown that it is possible to reproduce adequately the temperature profiles in Waldsee, a small meromictic lake in eastern Germany. Control simulations without the properly coupled geochemical and hydrodynamic model predicted a completely mixed lake due to the meteorological and hydrodynamic conditions. The measured profiles show a stable stratification due to groundwater inflow and Fe and Mn mineral dissolution/precipitation cycles. In order to reproduce temperature profiles, it is necessary to simulate the different geochemical processes and account for the dependence of density on the chemical composition of the water.

1. INTRODUCTION

Many pit lakes become meromictic during or after their formation, i.e. they are permanently stratified without seasonal or annual overturn (Boehrer and Schultze, 2006). Both subsurface inflows from aerated soils (von Rohden et al., 2009; Seebach et al., 2008) as well as geochemical transformations (Boehrer and Schultze, 2008) have been claimed to be responsible for sustaining the stratification. In addition, water-filled mine pits often have a small diameter-to-depth ratio compared to natural lakes, which is favourable for meromixis, (e.g. Castro and Moore, 2000; Sánchez et al., 2009, Hamblin et al., 1999). Some lakes become meromictic due to the accumulation of dissolved species, such as iron or sulfate, in the deepest lake layers due to precipitation/dissolution processes and groundwater inflows. Oxygen carried in from the atmosphere into the upper water layer (mixolimnion) promotes mineral oxidation and precipitation whereas the formation of an anoxic zone in the deep water (monimolimnion) at the bottom promotes the redissolution of the settling minerals. Both zones are separated by a strong gradient zone called chemocline. Mineral precipitation is largest in the chemocline where waters of different compositions mix and react. These phenomena lead to a strong stratification that can resist seasonal overturns. Under these conditions, lake hydrodynamics can be controlled by the biogeochemical processes.

The complexity of the hydrodynamic and geochemical processes requires complex models in order to predict the water quality and the effects of the remedial actions in pit lakes. Geochemical model predictions of pit lake chemistry are often employed by mine managers and regulators to assess the environmental effects of open pit mines. Model predictions are used to guide mine managers to develop site closure plans that minimize negative impacts (Miller et al. 1996, Castendyk and Webster-Brown, 2007b, Castendyk and Eary, 2009). In the case of existing open pit lakes, modelling tools can be very useful to test the effectiveness of different remedial actions before the elaboration of recovery plans.

Models have been used to simulate pit lake hydrodynamics. Balistrieri et al. (2006) and Castendyk and Webster-Brown (2007a) report model predictions of temperatures in pit lakes using DYRESM (Imberger and Patterson, 1981; CWR, 2006). Geochemical predictions of water chemistry of pit lakes are usually performed by assuming that lake waters are fully mixed and using hydrochemical codes such as PHREEQC (Parkhust and Appelo, 1999), EQ3/6 (Wolery et al., 1993) and CORE^{2D}V4 (Samper et al., 2003).

Hydrodynamic models such as those implemented in code DYRESM (Imberger and Patterson, 1981; Antenucci and

Imerito, 2003; CWR, 2006) in general provide a good representation of temperature and salinity profiles in lakes. A prognostication of meromixis has only been attempted for conservative salts (Böhrer et al 1998, Jellison et al 1998). However, the observed conditions in some meromictic lakes cannot be properly simulated with existing hydrodynamic codes. For these lakes, it is necessary to consider the density dependence on chemical composition, which must be calculated using geochemical models. None of the existing codes with coupling between hydrodynamics and geochemistry have been applied on meromictic pit lakes (Müller et al., 2008; Castendyk and Eary, 2009, Salmon et al. 2008 and Samper et al. 2008).

A novel equation for computing water density as a function of water chemical composition, developed in Helmholtz-Centre for Environmental Research-UFZ, has been presented recently by Moreira et al. (2009). This new equation is based on Chen and Millero (1986) and leads to a strong coupling of hydrodynamics and hydrogeochemistry. This equation has been implemented in DYCD-CORE (Moreira et al., 2009) and used to simulate the lake stratification and predict the temperature of the meromictic pit lake Waldsee.

2. COMPUTER CODE DYCD-CORE

A coupled hydrodynamic-geochemical code following the one-dimensional assumption, DYCD-CORE (Samper et al., 2008; Moreira et al., 2009), has been developed to model the hydrodynamics and geochemical evolution of pit lakes. This code incorporates the hydrodynamic and mixing processes of DYRESM (Dynamic Reservoir Simulation Model; Imberger and Patterson, 1981) and geochemical routines of the reactive transport code, $CORE^{2D}$ V4 (Samper et al., 2003), and the equation for computing water density from temperature and solute concentrations (Moreira et al., 2009). Particular characteristics (availability and modularity) of both codes make them suited for coupling and applying them to model acid pit lakes.

The coupled code DYCD-CORE can model the interaction between chemistry and hydrodynamics by calculating the geochemical composition of each layer and updating water density as a function of chemical composition. DYCD-CORE solves first the hydrodynamic processes by transporting chemical primary species and minerals. Geochemical calculations are performed by using the geochemical routines extracted from $CORE^{2D}$V4.

In order to consider the effect of the concentration of specific dissolved species in the density of the water in the monimolimnion, water densities are calculated from temperature and solute concentrations in DYCD-CORE instead of the original algorithm based on the equation of UNESCO (1983) implemented in DYRESM (CWR, 2006). Details of this coupling of hydrodynamics and hydrochemistry are provided by Moreira et al. (2009).

3. FIELD SITE AND FIELD DATA: PIT LAKE WALDSEE

Waldsee is a small shallow meromictic lake located near Döbern (Germany). The lake is located within a forest with significant sheltering against wind impact. The lake is closed and has a maximum depth of 4.7 m and a total area of 120x50m2 (Figure 1). Its catchment area is very small. The climate of the study area is characterized by an annual temperature range between -1.3 and 17.9 ºC (monthly averages) with a long term average temperature of 8.4ºC and a mean humidity close to 80 % (Seebach et al., 2008; Dietz et al. 2008).

Meteorological data are acquired at a station (Umweltanalytische Produkte, Cottbus, Germany) on the lake and data for cloud cover were collected in a nearby station of the German Meteorological Service (DWD).

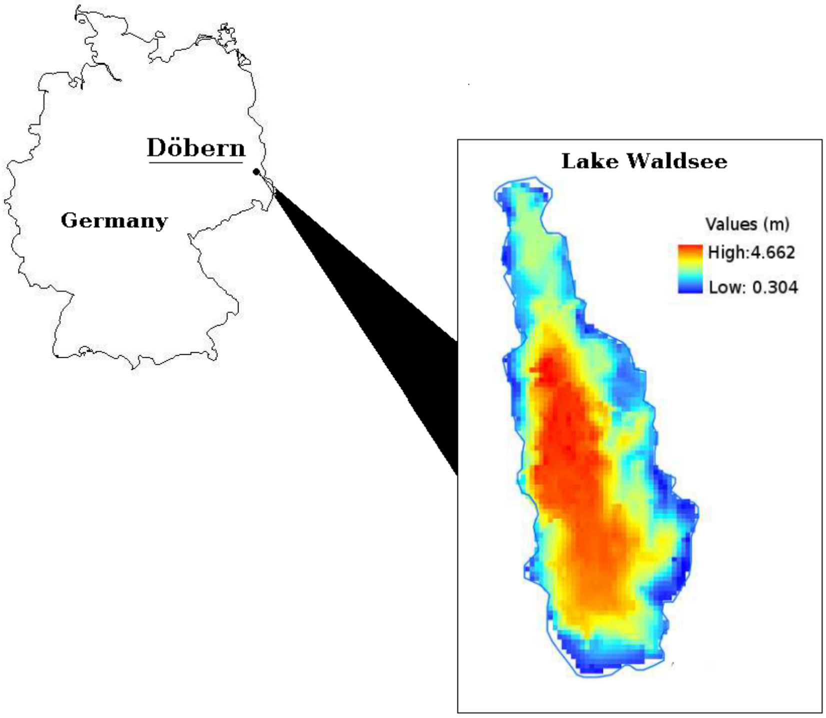

Figure 1. Location and morphometry of Waldsee

The lake shows a permanent stratification. The chemocline is established between 1m and 1.5m from the surface (Figure 2). A rise of the chemocline was observed during the cold season, indicating that probably groundwater flowed into the monimolimnion. Chemical reactions in the chemocline might also contribute to the fluctuations of the chemocline depth. Estimation of groundwater inflows and outflows were derived from tracer experiments and isotopic data by Seebach et al. (2008) and von Rohden et al. (2009). According to von Rohden et al. (2009), groundwater inflows are estimated to range from 4 to 12 m^3/d with a mean value of 8.2 m^3/d while groundwater outflows range from 0 to 12 m^3/d with a mean of 6.0 m^3/d.

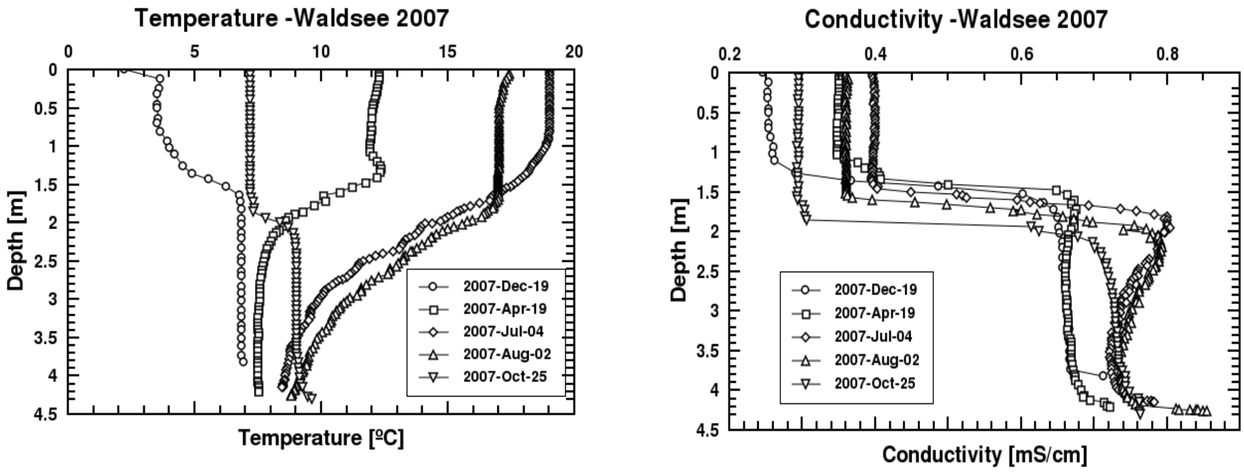

Figure 2. Temperature and conductivity profiles of Waldsee.

4. MODEL RESULTS AND DISCUSSION

Simulations were conducted over a period of 7 months covering the period between April 4th 2007 to October 10th 2007. The winter season was not simulated because the current version of DYRESM cannot deal with ice cover episodes which are common in Waldsee in the winter.

Groundwater was assumed to be the main inflow into the lake for modelling calculation. Its flux was assumed constant and was calibrated to a value of 8.5 m^3/day which leads to the best fit to measured profiles. The composition of inflowing groundwater was taken equal to the average value of available data from samples taken in the surrounding areas (Moreira et al., 2009).

Contour plots of model predictions of temperature in Waldsee are shown in Figures 3 and 4. The standard output of DYRESM (Figure 3) shows that the model with the UNESCO (1983) density equation predicts full mixing in the water column in terms of temperature and salinity. This happens even if the simulation is started with a stratified profile as it can be seen in the salinity contour plot; Figure 3b). This density equation uses the UNESCO (1983) equation and considers an average value of groundwater salinity equal to 0.7 psu. On the other hand, the model considering geochemical transformations and the modified water density equation predicts accurately the observed temperature stratification for almost all the simulation period (Figure 4, 5).

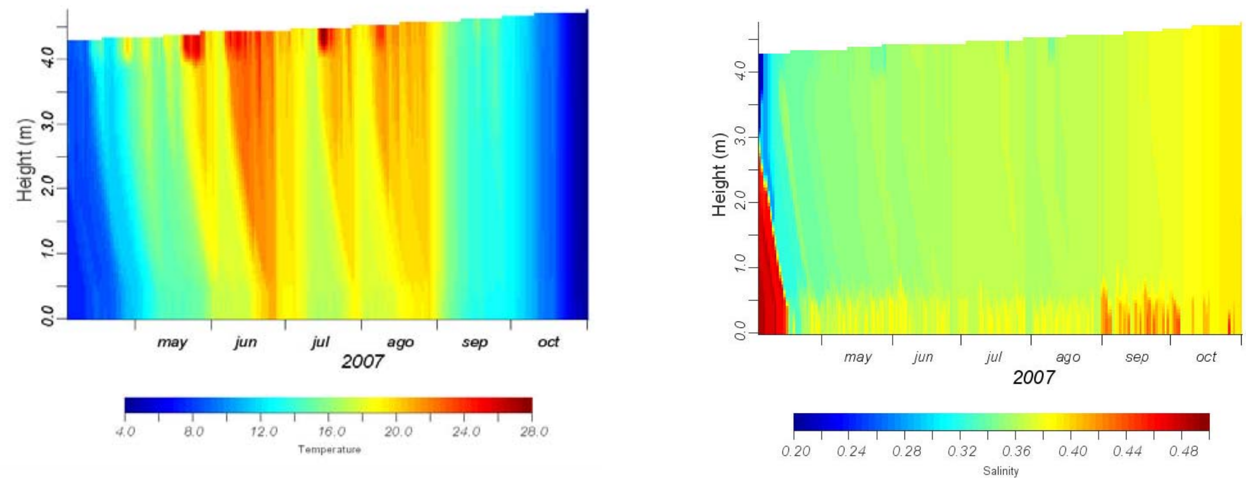

Figure 3. Contour plots of computed temperature (a) and salinity (b) with DYRESM by using the UNESCO (1983) water density equation. The main difference of the new algorithm to the UNESCO (1983) is the absence of the salinity term in the density equation. Instead of modelling salinity, a full geochemical model was run in each layer to calculate the total concentration of the dissolved species. These values were included in the calculation of the density. In this way, DYCD-CORE could reproduce temperature profiles observed in Waldsee (Figure 5) and could simulate the thermal inversion beginning in October. This is only possible by considering chemical composition in density calculations and by simulating geochemical processes in each one of the layers considered in the DYRESM model.

5. CONCLUSIONS

Geochemically-mediated meromixis cannot be predicted with existing hydrodynamic models because they do not account for the change in water density due to the chemical transformations. The successful application of a coupled hydrodynamic and geochemical model for meromictic lakes has been presented, in which the water density is computed from the water temperature and the concentrations of chemical solutes.

Although the current model improves the capabilities of existing models for meromictic lakes, it requires further improvements to account for settling materials, heat conduction, and dissolved oxygen. This model approach showed that modelling geochemically induced meromixis requires a strong coupling between chemical composition and density calculation, which includes a hydrodynamic model and a geochemical model, and that the geochemical transformations have to be properly evaluated in a density function. However, this approach also showed that the required knowledge is available. The coupling of the model yielded good results for Waldsee during the summer months of 2007.

6. ACKNOWLEDGEMENTS

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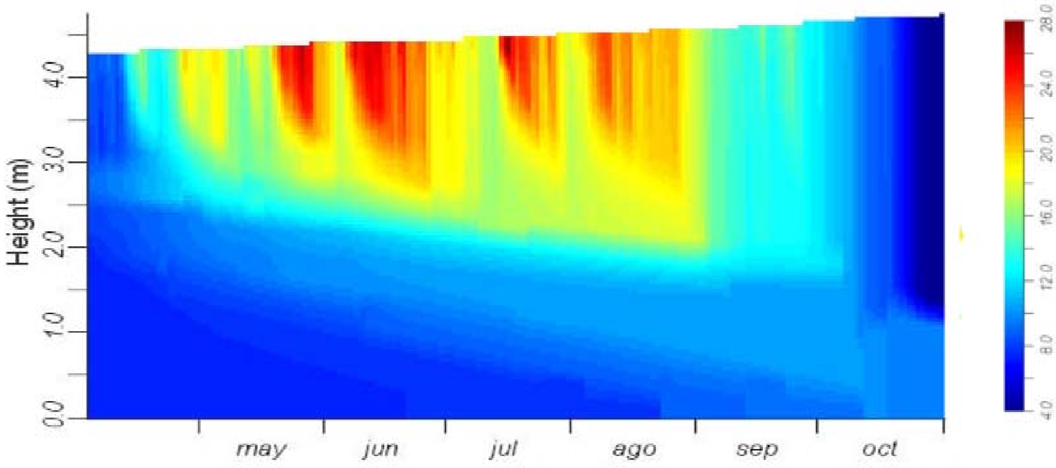

Figure 4. Contour plot of computed temperatures with DYCD-CORE by using the water density equation which accounts for the water chemical composition.

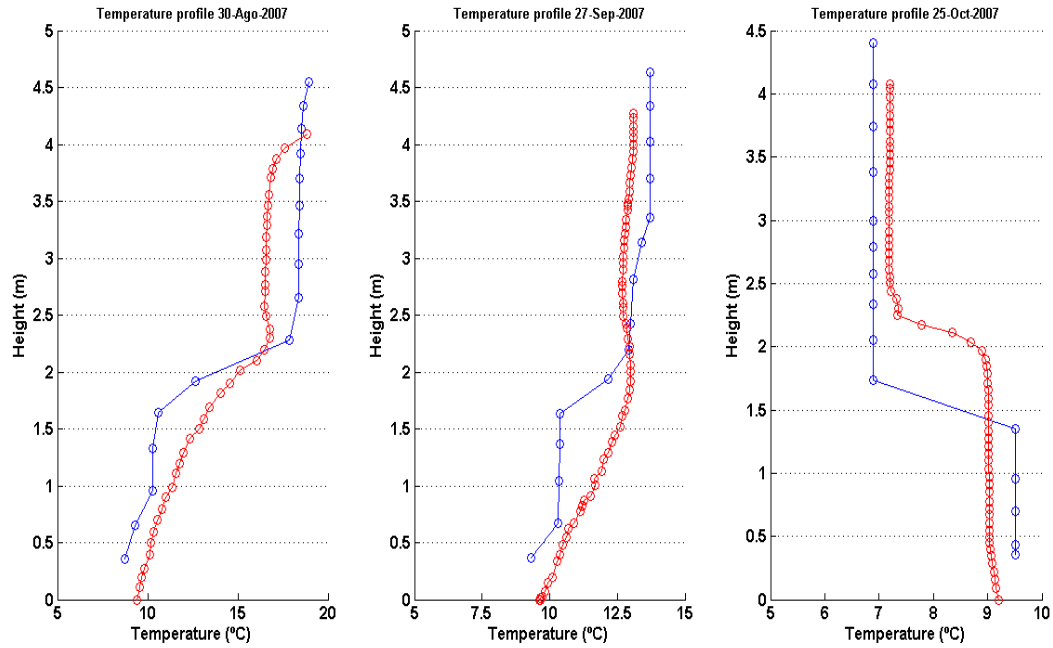

Figure 5. Comparison of measured temperature profiles (red symbols) and computed temperature profiles (blue symbols) in Waldsee.

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